Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material for "The Pyrolysis of 2-Methylfuran: A Quantum Chemical, Statistical Rate Theory and Kinetic Modelling Study"

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Contents

1 Potential Energy Surfaces for α-Carbene mediated Unimolecular Decomposition

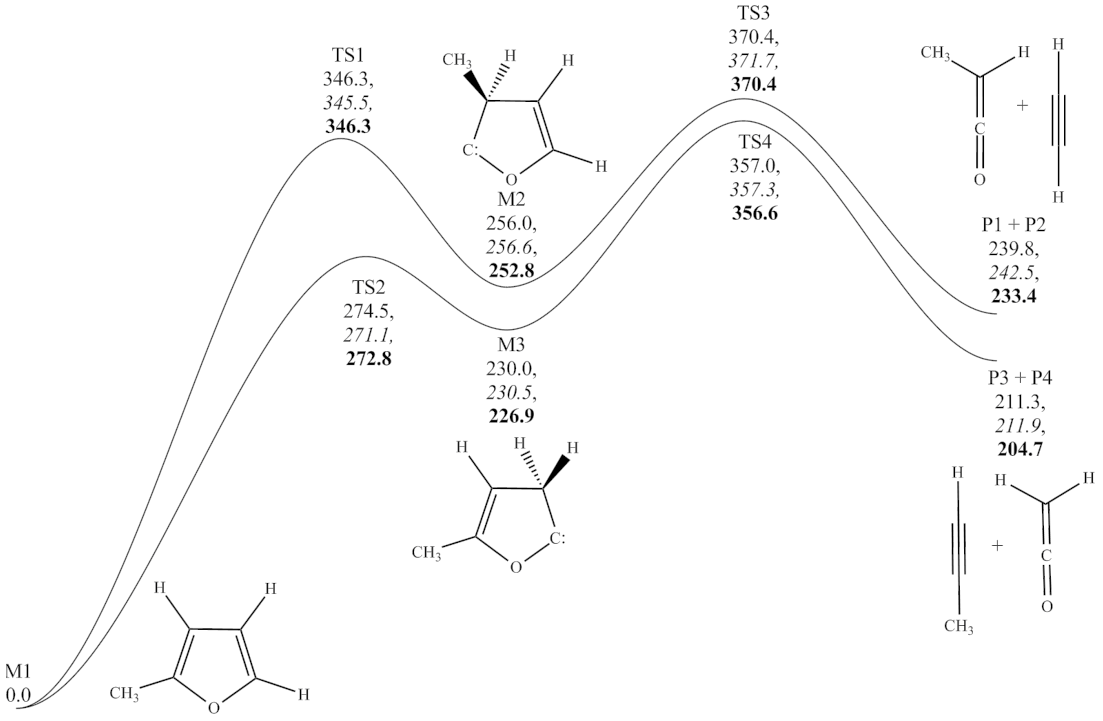

Figure 1: Potential energy surface for the formation and decomposition of α-carbenes. CBS-QB3, *CBS-APNO* and **G3** Energies in kJ mol^{-1} at 0 K relative to 2-methylfuran.

Figure 1 delineates the potential energy surfaces for the decomposition of 2-methylfuran through α-carbene intermediates. Based on CBS-QB3 calculations, a 2 $\rightarrow$ 3 methyl shift to form a singlet α-carbene (**M2**) occurs with a transition state lying 346.3 kJ mol^{-1} above the reactant in a reaction which is endothermic by 256.0 kJ mol^{-1}, in good agreement with values computed for the analagous 25DMF [1] and those of Davis for 2MF [2]. The carbene subsequently decomposes in a mildly exothermic ($-$16.2 kJ mol^{-1}) reaction forming methyl ketene ($CH_3-CH=C=O$) and acetylene ($HC\equiv CH$) with the transition structure lying 114.5 kJ mol^{-1} above the carbene intermediate and 370.4 kJ mol^{-1} above 2MF.

The formation of an α-carbene (**M3**) from a 5 $\rightarrow$ 4 hydrogen transfer proceeds through a barrier of only 274.5 kJ mol^{-1} based on a CBS-QB3 computation with a reaction enthalpy of 230 kJ mol^{-1}. Decomposition to $CH_2=C=O$ and $HC\equiv C-CH$ follows through a barrier 127.0 kJ mol^{-1} above the carbene and 357.0 kJ mol^{-1} above 2MF. The energetics of this multistep process are in excellent agreement with G3(MP2), CASPT2 and CBS-QB3 calculations carried out for the similar process in furan [3,4].**TS3** and **TS4** correspond to those for Diels-Alder type reactions and multi-reference effects may be of importance. T1 diagnostics were therefore computed and found to be 0.019 for **TS3** and 0.018 for **TS4**, thus indicating that single-reference methods used suffice. The computed decomposition rate constants for the α-carbenes (k_3 and k_4) are in excellent agreement as one might expect, given their similar decomposition mechanism and products.

Methyl ketene was identified in the low pressure flames of 25DMF, which is formed along with $HC\equiv C-CH$, in an effectively identical process to the above [1]. Based on the computed energetics and kinetics of this process however, its production from 2MF and 25DMF is insignificant.

2 Potential Energy Surfaces for Hydrogen Atom Addition at C-3 and C-4.

Figure 2 describes the potential energy surface for hydrogen atom addition at C-3 of 2MF. Despite the rate constant for addition at C-3 being competitive with addition at C-2, the addition forming **M28** is much less exothermic than that forming **M17** *via* $\dot{H}$ atom addition at C-2, with the latter capable of undergoing resonance stabilisation to delocalise the radical formed.

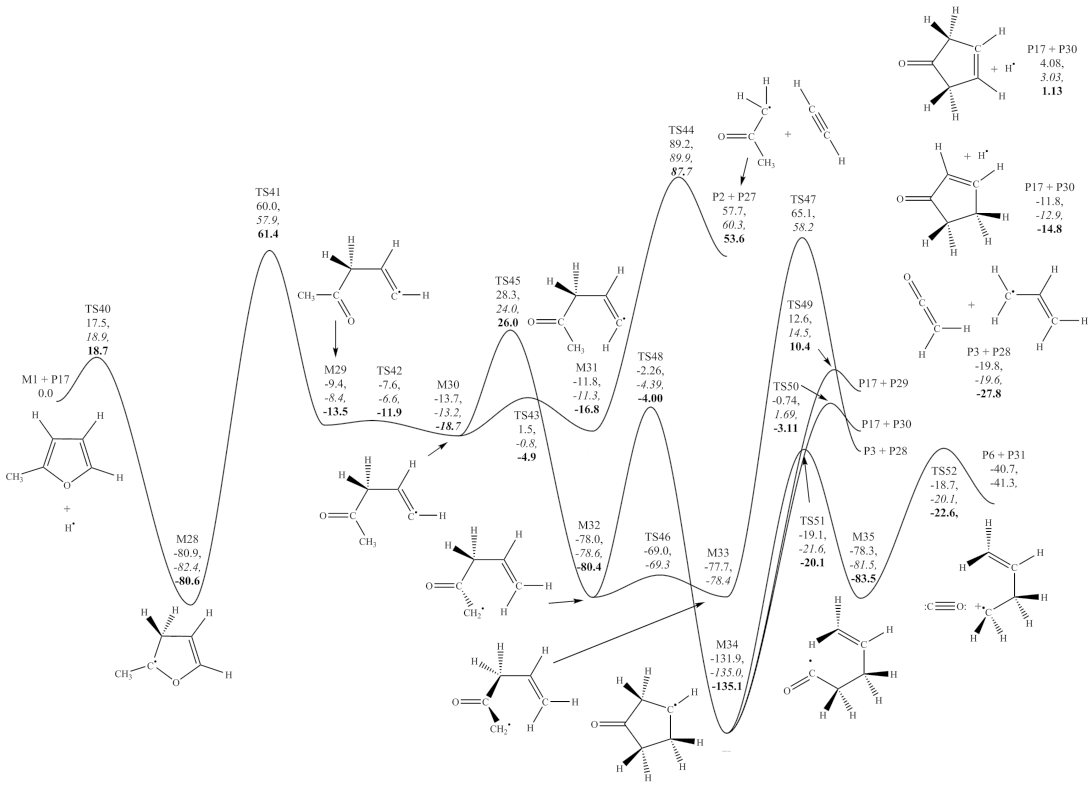

Figure 2: Potential energy surface for hydrogen atom addition at carbon 3 of 2-methylfuran. CBS-QB3, *CBS-APNO* and **G3** energies in kJ mol^{-1} at 0 K relative to reactants.

In turn the ring opening reaction of **M28** through a barrier of 141.1 ± 0.9 kJ mol^{-1} (**TS41**) is much less facile than those of **M17** (k_{26} and k_{30}). This is clearly a result of the vinylic nature of **M28**, with the process being endothermic by 70.9 ± 3.5 kJ mol^{-1}. The ring opening of **M17** is shown to be exothermic (−2.90 ± 1.3 kJ mol^{-1}), with the radical formed being allylic in nature.

Table 1: Arrhenius coefficients of high-pressure limiting rate constants for for reactions relevant to hydrogen atom addition at C-3 of 2-methylfuran. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/R)$, AT^n (s^{-1}), E_a/R (K).

No.	Reaction	A	n	E_a/R (K)
k_{41}	M28 → M29	2.92×10^{11}	0.66	16915.
k_{42}	M29 → M30	1.50×10^{09}	0.90	−65.
k_{43}	M30 → M31	2.28×10^{09}	1.22	1524.
k_{44}	M31 → P2 + P27	8.98×10^{10}	1.00	12619.
k_{45}	M30 → M32	6.08×10^{02}	2.58	2663.
k_{46}	M32 → M33	6.36×10^{09}	0.64	626.
k_{47}	M33 → P3 + P28	1.38×10^{09}	1.31	17053.
k_{48}	M32 → M34	2.66×10^{08}	0.82	8272.
k_{49}	M34 → P17 + P29	1.55×10^{10}	1.02	17412.
k_{50}	M34 → P17 + P30	1.74×10^{10}	0.98	15751.
k_{51}	M34 → M35	1.94×10^{12}	0.26	13712.
k_{52}	M35 → P6 + P31	9.41×10^{12}	0.42	7590.

A similar scenario arises upon Ḣ atom addition at C-4, Figure 3, where ring opening of the adduct proceeds through a barrier of 145.7 ± 2.2 kJ mol^{-1} with the formation of a secondary vinylic radical (**M37**) being endothermic by 80.1 ± 2.5 kJ mol^{-1}. Computed rate constants for ring opening reactions of C-3 and C-4 Ḣ atom addition adducts are in excellent agreement, k_{41} and k_{54} respectively.

The fate of these acyclic intermediates is of a lesser importance than those formed from addition at C-2, as β-scission of a C–H bond to reform 2MF and hydrogen atom dominates over ring opening based on our computed

Table 2: Arrhenius coefficients of high-pressure limiting rate constants for for reactions relevant to hydrogen atom addition at C-4 of 2-methylfuran. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/R)$, AT^n (s^{-1}), E_a/R (K).

No.	Reaction	A	n	E_a/R (K)
k_{54}	M36 → M37	2.98×10^{12}	0.39	17520.
k_{55}	M37 → M38	5.81×10^{08}	0.93	−334.
k_{56}	M38 → P4 + P32	4.63×10^{10}	0.98	11385.
k_{57}	M37 → M39	4.08×10^{12}	−0.01	615.
k_{58}	M39 → M40	1.41×10^{09}	0.92	183.
k_{59}	M40 → P6 + P33	1.11×10^{11}	0.64	3744.

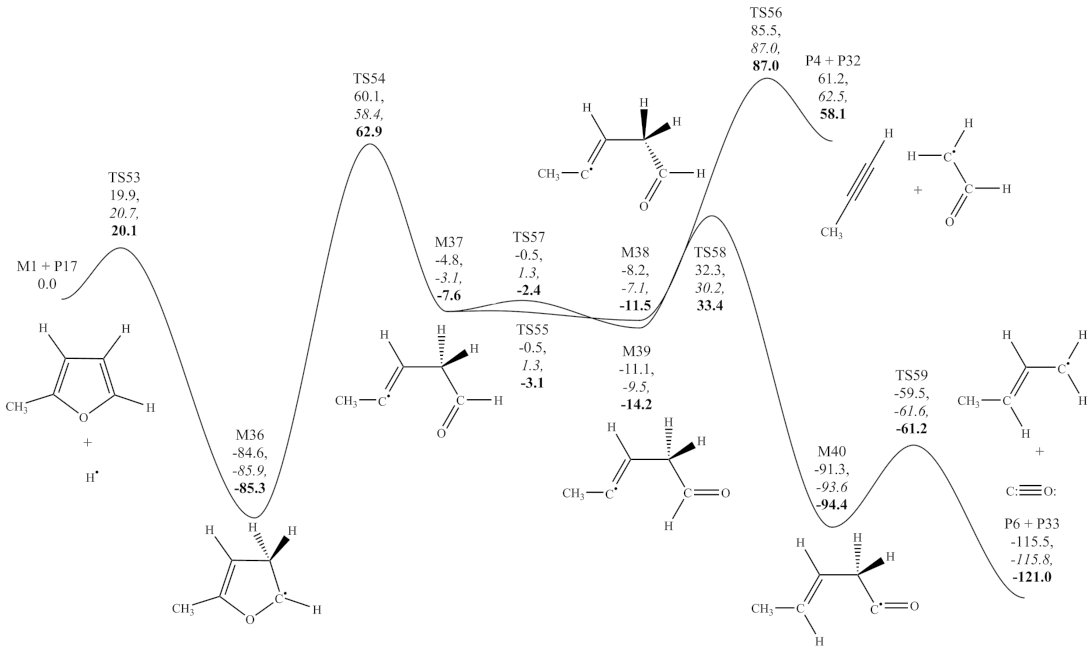

Figure 3: Potential energy surface for hydrogen atom addition at carbon 4 of 2-methylfuran. CBS-QB3, *CBS-APNO* and **G3** energies in kJ mol^{-1} at 0 K relative to reactants.

kinetics and thermochemistry. As a result, RRKM/ME analysis has not been applied to addition at C-3 and C-4, although the fate of the ring opening products has nontheless been investigated to gain further mechanistic information into the decomposition pathways of furanic species.

M29 can undergo isomerisation *via* a 1→5 hydrogen shift to form a more stable primary radical (**M32**) with the ultimate formation of ketene and an allyl radical through a transition state (**TS47**) at 61.7 ± 4.9 kJ mol^{-1} above 2MF and hydrogen atom. The formation of acetylene and the acetonyl radical is also possible *via* **TS44**, and the rate constant for its formation from **M31** is seen to become competitive with that of the hydrogen transfer reaction (k_{47}) at temperatures above 1600 K. Ring closing to form a cyclopenteneone radical (**M34**), which can occur with a computed barrier of 113.8 ± 1.1 kJ mol^{-1}, is unlikely despite the modest activation energy for the process.

M37 can form a more stable aldehydic radical (**M40**) *via* hydrogen transfer through **TS58**. The subsequent decarbonylation reaction forming CO and $\dot{C}H_2$—CH=CH—CH_3 through **TS59** is quite quite rapid. The endothermic formation of CH≡C—CH and $\dot{C}H_2$—CH=O radicals can also occur and despite the large barrier (95.4 ± 2.7 kJ mol^{-1}) when compared with the hydrogen transfer reaction, its formation should become competitive above 1500 K.

3 Influence of $\langle \Delta E_d \rangle$ on RRKM/ME Derived $k(T, p)$

In order to evaluate the influence of $\langle \Delta E_d \rangle$ on the computed temperature- and pressure-dependent rate constants, test calculations with $\langle \Delta E_d \rangle$ = 500 cm^{-1} and 2000 cm^{-1} were carried out on some potential energy surfaces. The pressure chosen was 2.5 atm., equivalent to the average pressure in the shock tube pyrolysis study of Lifshitz *et al.*.

The results show a small variation in the computed rate constants for the unimolecular decomposition reactions of 2-methylfuran (Figures 4–7), with the largest variations observed at the highest temperatures studied (2000 K) where fall-off in the high-pressure limiting rate constants is greatest. Relative to the $\langle \Delta E_d \rangle$ = 1000 cm^{-1} computations, the rate constants computed with $\langle \Delta E_d \rangle$ = 500 cm^{-1} and 2000 cm^{-1} vary by ≈ a factor of two at 2000 K. Under the conditions of Lifshitz *et al.* study (1200–1500 K, once their temperature profile is corrected), the variation in the computed rate constants with the various values of $\langle \Delta E_d \rangle$ chosen is minimal, and the rate constants are close to the high-pressure limiting rate constants in all cases.

Test calculations were also carried out on the reaction 2-methylfuran + hydrogen atom → products (C-2 addition, Figures 8–11). The largest variation observed in the computed rate constants was ≈ a factor of 7 at 600 K for the reaction 2-methylfuran + hydrogen atom → **P9** (formyl radical) + **P24** (1,3-butadiene) with $\langle \Delta E_d \rangle$ = 500 cm^{-1}. However, it should be noted that this is a very minor reaction pathway whose branching ratio is ≈ 5 × 10^{-08} under these conditions (600 K, 2.5 atm, $\langle \Delta E_d \rangle$ = 1000 cm^{-1}). The uncertainty in this reaction pathway due to the choice of $\langle \Delta E_d \rangle$ is of little concern with respect to kinetic modelling studies. For all other reactions pathways, reducing $\langle \Delta E_d \rangle$ to 500 cm^{-1} led to a variation of ≈ a factor of 2–3 from the rate constants computed with $\langle \Delta E_d \rangle$ = 1000 cm^{-1}. Increasing $\langle \Delta E_d \rangle$ to 2000 cm^{-1} resulted in a variation in the computed rate constants of ≈ a factor of 2.

3.1 Unimolecular Decomposition of 2-Methlyfuran

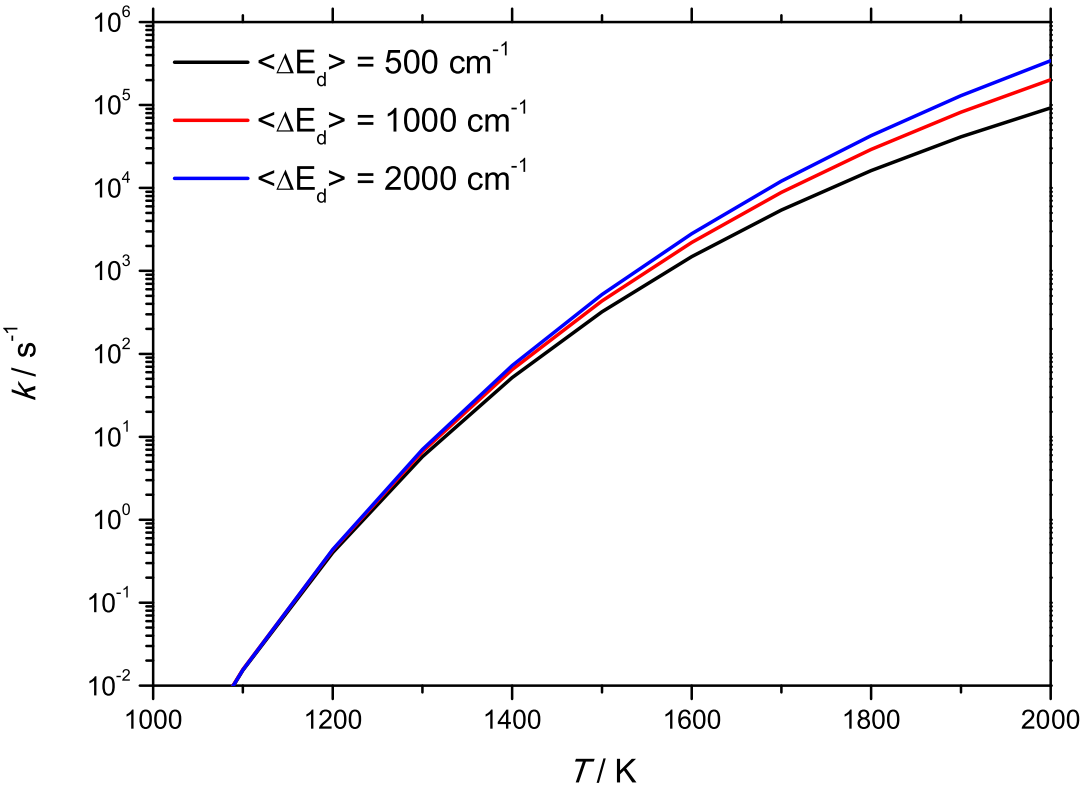

Figure 4: Influence of altering $\langle \Delta E_d \rangle$ ± a factor of 2 on the computed rate constant for the reaction 2-methylfuran → **P3** + **P4** (ketene + propyne) at a pressure of 2.5 atm.

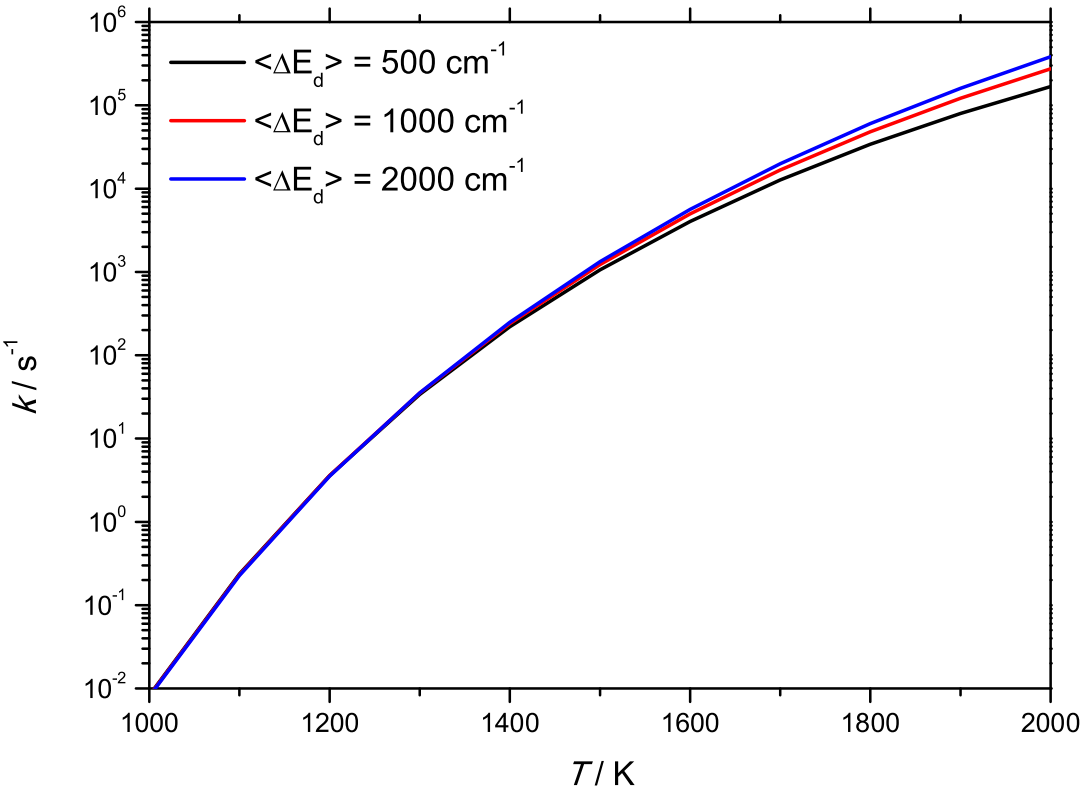

Figure 5: Influence of altering $\langle \Delta E_d \rangle$ ± a factor of 2 on the computed rate constant for the reaction 2-methylfuran → **M6** (2,3-pentadiene-1-al) at a pressure of 2.5 atm.

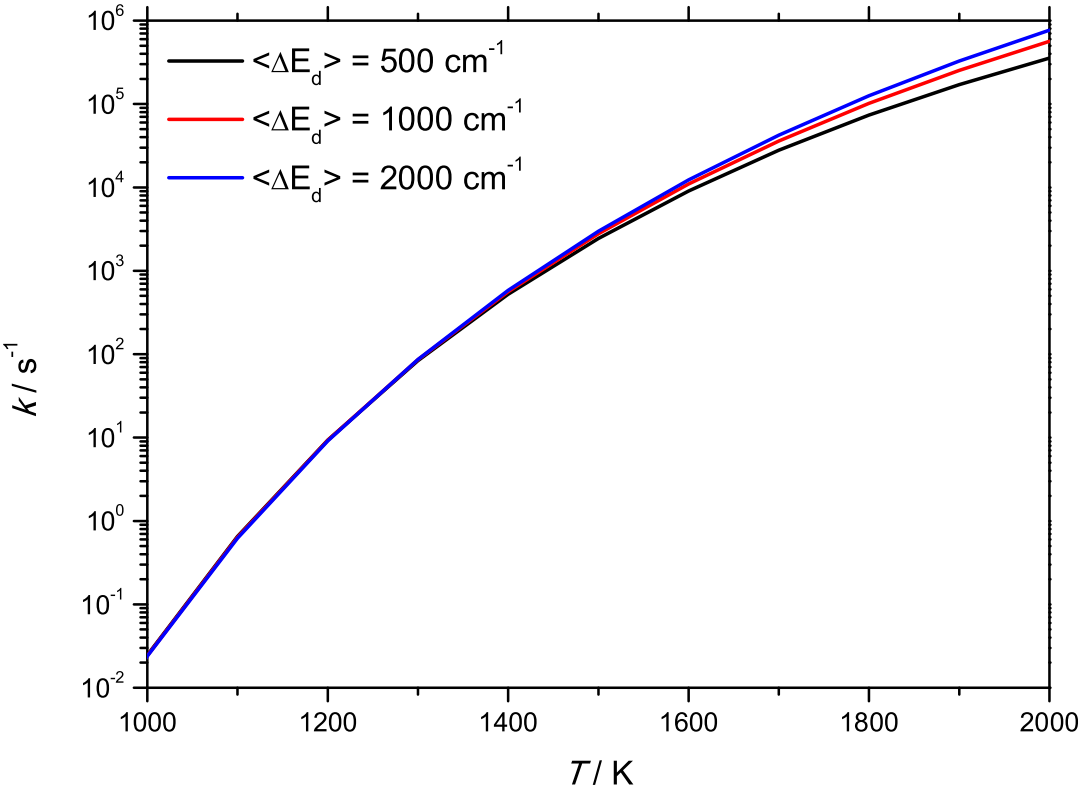

Figure 6: Influence of altering $\langle \Delta E_d \rangle$ ± a factor of 2 on the computed rate constant for the reaction 2-methylfuran → **M9** (3,4-pentadiene-2-one) at a pressure of 2.5 atm.

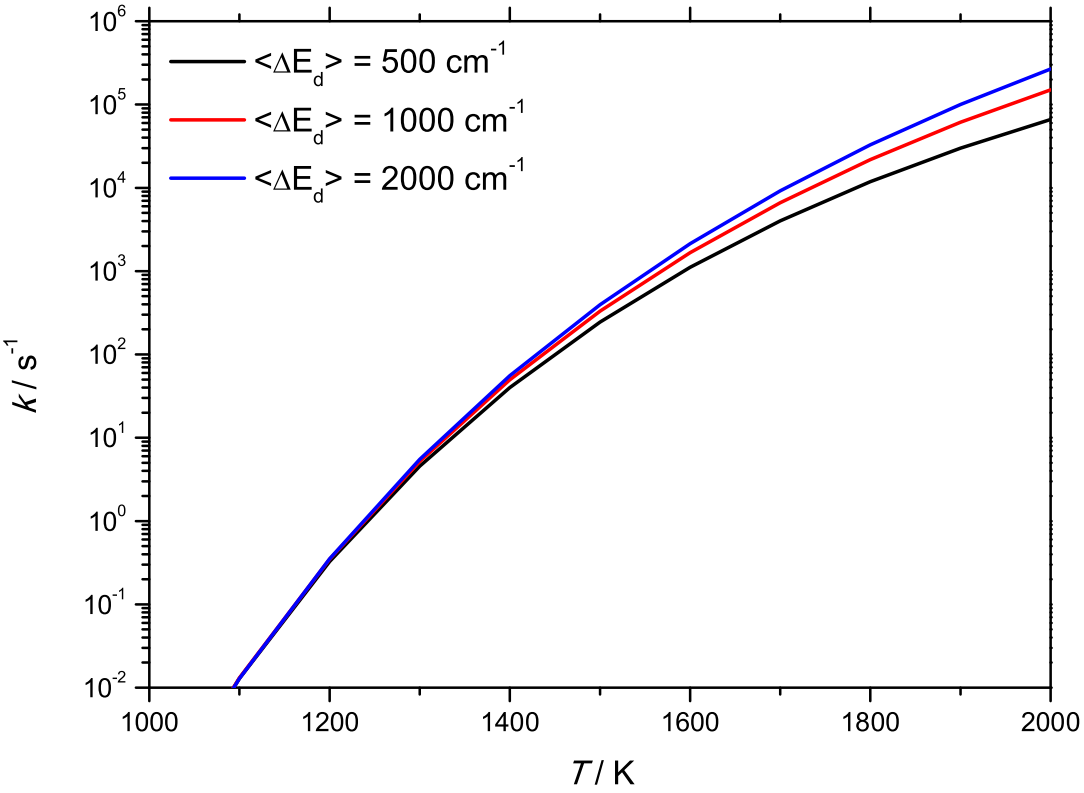

Figure 7: Influence of altering $\langle \Delta E_d \rangle$ ± a factor of 2 on the computed rate constant for the reaction 2-methylfuran → **M10** + **P17** (2-furanylmethyl + hydrogen atom) at a pressure of 2.5 atm.

3.2 Hydrogen Atom Addition at Carbon 2 of 2-Methylfuran

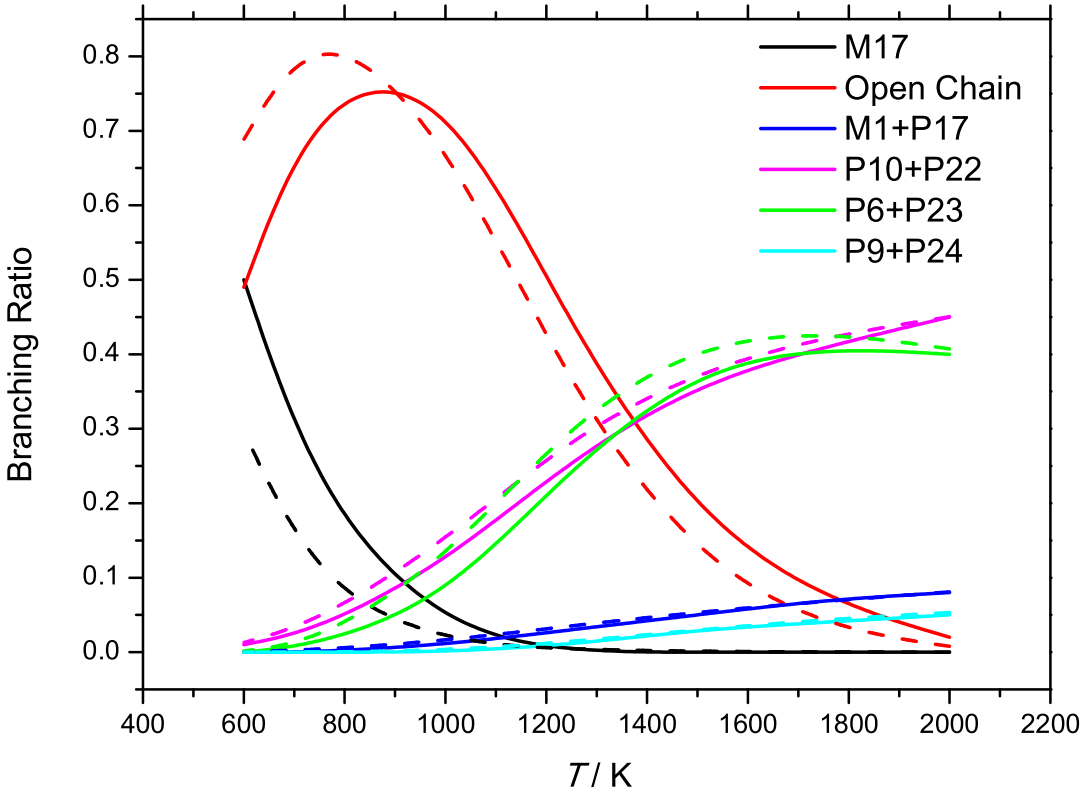

Figure 8: Computed product branching ratios at 2.5 atm. for the reaction 2-methylfuran + hydrogen atom (C-2 addition) → products. $\langle \Delta E_d \rangle$ = 2000 cm^{-1} (—); $\langle \Delta E_d \rangle$ = 500 cm^{-1} (– –).

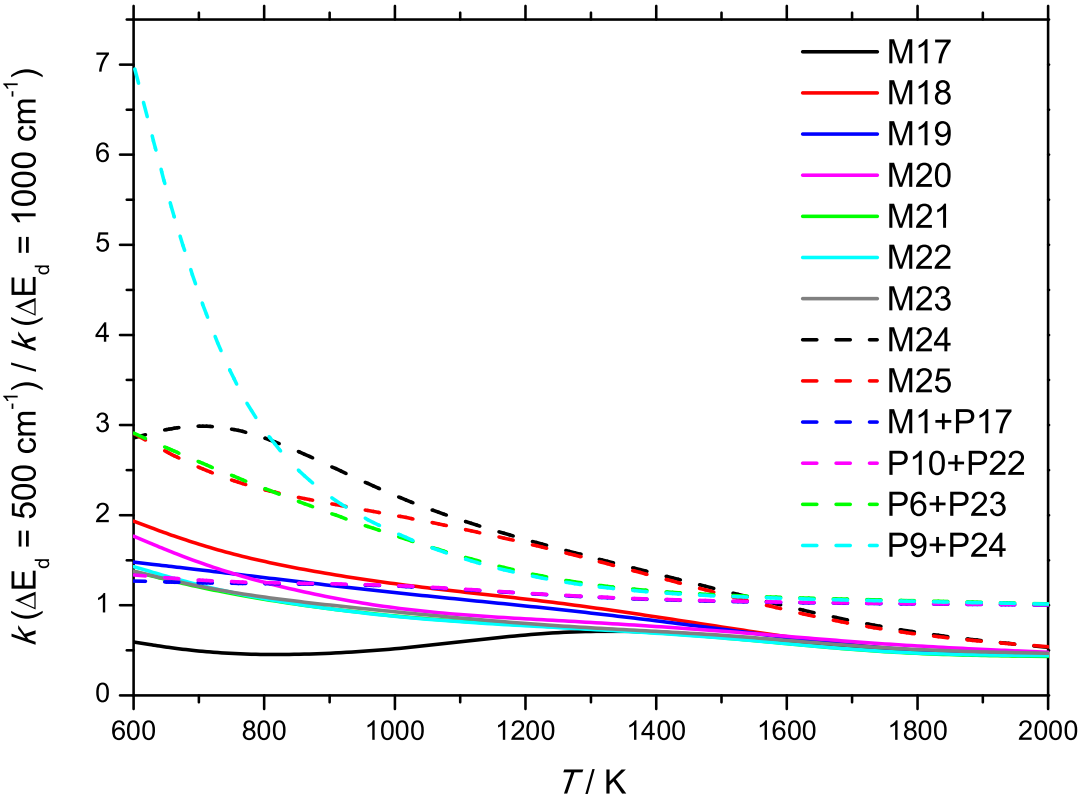

Figure 9: Ratio of computed rate constants for the reaction 2-methylfuran + hydrogen atom → products at 2.5 atm., with $\langle \Delta E_d \rangle$ = 500 cm^{-1} and $\langle \Delta E_d \rangle$ = 1000 cm^{-1}.

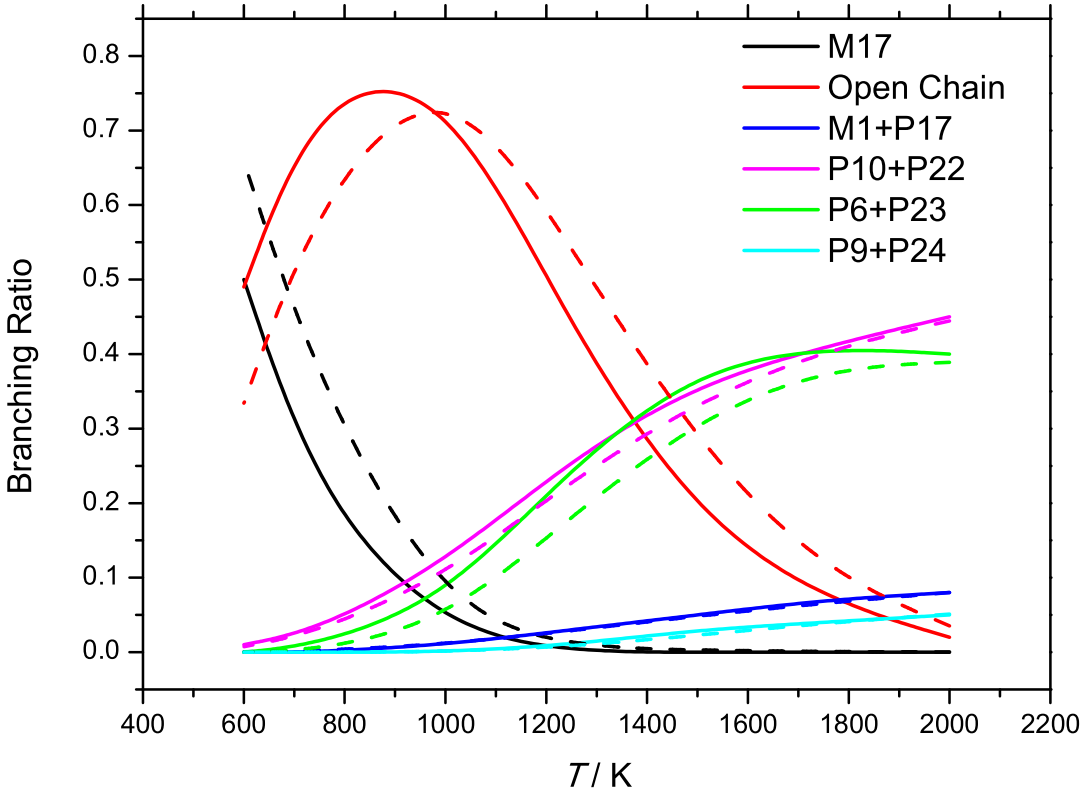

Figure 10: Computed product branching ratios at 2.5 atm. for the reaction 2-methylfuran + hydrogen atom (C-2 addition) → products. $\langle \Delta E_d \rangle$ = 2000 cm^{-1} (—); $\langle \Delta E_d \rangle$ = 2000 cm^{-1} (– –).

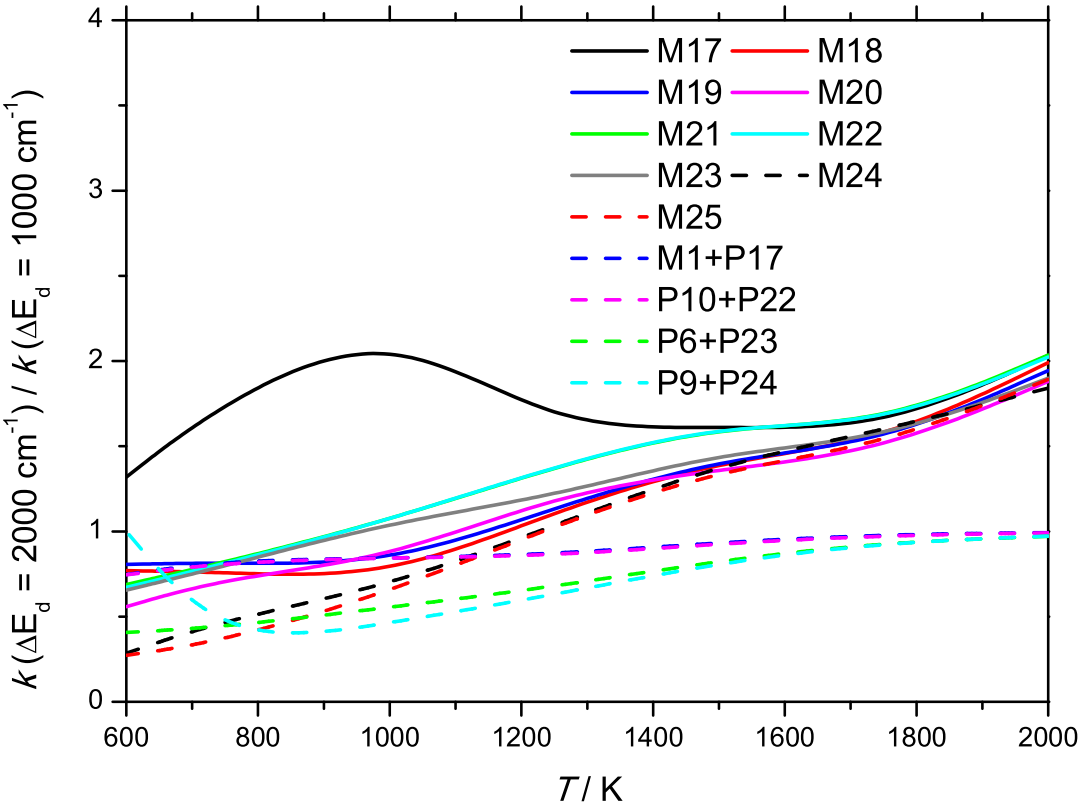

Figure 11: Ratio of computed rate constants for the reaction 2-methylfuran + hydrogen atom → products at 2.5 atm., with $\langle \Delta E_d \rangle$ = 2000 cm^{-1} and $\langle \Delta E_d \rangle$ = 1000 cm^{-1}.

4 Pressure Dependent Rate Constants from RRKM/ME Calculations

4.1 Chemkin-PRO Compatible PLOG Rate Constants

Table 3: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the unimolecular decomposition of 2-methylfuran and related intermediates. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
M1 → M3	0.01	5.12E+66	-15.39	97801
	0.1	1.25E+57	-12.47	93815
	1	4.11E+38	-7.10	82916
	2.5	9.13E+31	-5.19	78799
	10	4.49E+23	-2.80	73549
	100	3.41E+15	-0.48	68305
M3 → P3 + P4	0.01	3.51E+48	-10.26	45743
	0.1	4.87E+54	-11.66	53545
	1	4.56E+48	-9.71	52461
	2.5	9.25E+43	-8.31	50120
	10	1.15E+36	-6.01	45637
	100	3.68E+25	-2.98	39180
M1 → M6	0.01	2.17E+72	-17.14	105418
	0.1	2.77E+63	-14.37	102515
	1	3.81E+43	-8.58	91138
	2.5	1.10E+36	-6.41	86543
	10	1.98E+26	-3.60	80450
	100	1.95E+16	-0.74	74027
M1 → M9	0.01	4.07E+70	-16.58	102965
	0.1	2.59E+61	-13.75	99646
	1	9.73E+41	-8.09	88398
	2.5	5.63E+34	-6.01	83964
	10	3.26E+25	-3.35	78165
	100	1.55E+16	-0.68	72168
M1 → M10 + P17	0.01	2.89E+92	-22.81	127594
	0.1	1.06E+87	-20.85	128912
	1	1.42E+65	-14.34	117910
	2.5	2.15E+55	-11.48	112302
	10	1.63E+41	-7.39	103833
	100	1.97E+24	-2.53	93217
M6 → P5 + P6	0.01	7.52E+57	-13.07	70107
	0.1	2.45E+45	-9.31	64145
	1	2.26E+34	-6.06	58261
	2.5	1.52E+30	-4.84	55869
	10	9.55E+24	-3.32	52837
	100	3.45E+18	-1.46	48961
M6 → P6 + P7	0.01	1.82E+82	-19.88	99104
	0.1	1.35E+66	-14.92	92199
	1	5.20E+48	-9.73	83042
	2.5	3.19E+42	-7.90	79592
	10	4.14E+35	-5.86	75903
	100	3.60E+27	-3.48	71654

Table 3: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the unimolecular decomposition of 2-methylfuran and related intermediates. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
M9 → P3 + P4	0.01	4.63E+98	-24.44	115044
	0.1	5.48E+87	-20.97	111832
	1	2.57E+73	-16.59	105899
	2.5	1.72E+67	-14.74	102980
	10	7.68E+57	-11.97	98229
	100	2.61E+43	-7.73	90132
M9 → P13 + P14	0.01	9.56E+85	-21.57	106694
	0.1	2.05E+76	-18.47	104322
	1	2.69E+62	-14.22	98759
	2.5	1.40E+56	-12.33	95815
	10	2.65E+46	-9.44	90900
	100	1.02E+31	-4.93	82324

Table 4: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the unimolecular decomposition of 2-furanylmethyl radical and related intermediates. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
M10 → M11	0.01	4.49E+61	-14.18	64492
	0.1	5.05E+59	-13.42	65593
	1	4.62E+50	-10.65	61945
	2.5	4.98E+45	-9.17	59475
	10	1.88E+37	-6.70	54959
	100	7.14E+23	-2.79	47253
M11 → P17 + P18	0.01	3.18E+29	-7.07	46866
	0.1	4.47E+47	-11.61	58081
	1	7.77E+62	-15.19	71711
	2.5	1.31E+66	-15.81	76149
	10	3.54E+65	-15.23	79663
	100	5.91E+47	-9.66	73572
M11 → M12	0.01	1.92E+23	-3.09	12414
	0.1	1.36E+24	-3.27	13699
	1	9.86E+22	-2.88	13663
	2.5	1.01E+22	-2.58	13262
	10	1.11E+20	-2.00	12301
	100	3.10E+16	-0.96	10330
M12 → M13	0.01	2.29E+35	-7.31	30103
	0.1	7.37E+40	-8.62	35996
	1	1.60E+41	-8.48	38761
	2.5	2.25E+39	-7.87	38506
	10	2.28E+34	-6.34	36515
	100	1.01E+23	-2.98	30549
M13 → M14	0.01	5.27E+27	-4.36	17157
	0.1	4.79E+24	-3.47	15507
	1	2.97E+20	-2.25	13109
	2.5	3.12E+18	-1.68	11914
	10	3.55E+15	-0.83	10112
	100	3.02E+11	0.33	7517
M14 → P6 + P19	0.01	2.72E+50	-10.60	38351
	0.1	2.76E+56	-12.06	45564
	1	6.26E+55	-11.63	48704
	2.5	1.11E+46	-8.82	42672
	10	2.95E+42	-7.69	42310
	100	1.33E+27	-3.25	33671
M13 → M15	0.01	8.53E+34	-6.33	24268
	0.1	9.35E+30	-5.17	22282
	1	1.15E+25	-3.45	19007
	2.5	1.33E+22	-2.60	17242
	10	6.13E+17	-1.35	14614
	100	3.37E+11	0.44	10639
M15 → M16	0.01	1.30E+34	-6.30	24079
	0.1	1.62E+30	-5.15	22128
	1	2.36E+24	-3.45	18897
	2.5	2.95E+21	-2.61	17154

Table 4: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the unimolecular decomposition of 2-furanylmethyl radical and related intermediates. $k(\mathrm{s}^{-1}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
	10	1.55E+17	-1.38	14559
	100	1.10E+11	0.38	10649
M16 → P17 + P20	0.01	2.21E+77	-18.51	85730
	0.1	6.80E+81	-19.49	92440
	1	3.18E+73	-16.76	91956
	2.5	7.85E+58	-12.53	83194
	10	4.40E+50	-9.98	80861
	100	3.51E+23	-2.13	65606

Table 5: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the chemically activated recombination of hydrogen atom with 2-methylfuran at carbon 2. $k(\mathrm{cm^3 mol^{-1} s^{-1}}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
M1 + P17 → P10 + P22	0.01	5.93E+17	-1.13	10160
	0.1	6.31E+15	-0.49	10818
	1	6.25E+15	-0.44	12156
	2.5	6.28E+15	-0.43	12614
	10	7.55E+15	-0.43	13614
	100	2.47E+21	-1.92	19575
M1 + P17 → P6 + P23	0.01	3.28E+24	-3.07	13756
	0.1	1.22E+31	-4.83	20365
	1	3.52E+33	-5.39	25717
	2.5	6.30E+31	-4.83	26504
	10	1.69E+27	-3.43	27006
	100	1.27E+17	-0.43	26869
M1 + P17 → P9 + P24	0.01	4.08E+34	-6.02	26367
	0.1	2.42E+34	-5.81	29573
	1	9.29E+52	-10.88	46873
	2.5	4.08E+52	-10.63	50324
	10	1.52E+52	-10.34	55297
	100	3.16E+21	-1.47	43388
M1 + P17 → M17	0.01	9.42E+64	-16.86	22009
	0.1	4.08E+65	-16.74	23378
	1	1.91E+39	-8.86	8696
	2.5	1.53E+38	-8.43	8247
	10	6.02E+43	-9.88	11916
	100	2.32E+61	-14.59	24263
M1 + P17 → M18	0.01	2.70E+78	-20.34	33228
	0.1	6.04E+77	-19.70	36451
	1	1.25E+55	-12.72	27383
	2.5	3.26E+53	-12.08	28627
	10	6.16E+44	-9.38	25899
	100	3.31E+30	-5.02	21526
M1 + P17 → M19	0.01	1.39E+75	-19.25	30503
	0.1	6.80E+76	-19.31	34924
	1	6.02E+54	-12.51	26305
	2.5	9.25E+49	-10.96	25364
	10	9.05E+41	-8.47	22964
	100	1.32E+29	-4.53	19323
M1 + P17 → M21	0.01	2.78E+68	-17.43	23706
	0.1	2.14E+73	-18.47	28937
	1	6.73E+58	-13.83	24722
	2.5	2.87E+55	-12.69	24563
	10	1.01E+51	-11.17	24850
	100	1.98E+39	-7.45	23483
M1 + P17 → M22	0.01	4.29E+67	-17.15	23482
	0.1	1.30E+72	-18.06	28630
	1	2.15E+58	-13.63	24825
	2.5	2.21E+55	-12.60	24917

Table 5: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the chemically activated recombination of hydrogen atom with 2-methylfuran at carbon 2. $k(\mathrm{cm^3 mol^{-1} s^{-1}}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
	10	9.14E+50	-11.10	25255
	100	9.96E+38	-7.30	23686
M1 + P17 → M23	0.01	7.53E+72	-18.62	26476
	0.1	1.17E+77	-19.39	32694
	1	7.07E+58	-13.68	26972
	2.5	4.14E+51	-11.46	24431
	10	1.98E+45	-9.45	23414
	100	3.59E+38	-7.20	24843
M1 + P17 → M24	0.01	3.01E+70	-18.18	32181
	0.1	1.20E+91	-23.67	48986
	1	1.58E+77	-19.09	48486
	2.5	4.57E+69	-16.73	46964
	10	4.01E+51	-11.33	39795
	100	4.54E+48	-10.01	48245
M1 + P17 → M25	0.01	9.09E+78	-20.71	37095
	0.1	6.30E+92	-24.28	49388
	1	1.90E+73	-18.04	45934
	2.5	1.94E+69	-16.70	46393
	10	7.29E+58	-13.45	44651
	100	5.86E+13	-0.26	23754

Table 6: Chemkin-PRO PLOG format pressure- (atm) and temperature-dependent rate constants for the chemically activated recombination of hydrogen atom with 2-methylfuran at carbon 5. $k(\mathrm{cm^3 mol^{-1} s^{-1}}) = AT^n \exp(-E_a/RT)$.

Reaction	p (atm)	A	n	E_a (cal/mol)
M1 + P17 → P10 + P34	0.01	1.07E+39	-6.67	30846
	0.1	1.50E+47	-8.88	38568
	1	5.03E+47	-8.89	42758
	2.5	8.28E+44	-8.04	42837
	10	6.18E+36	-5.65	40637
	100	1.44E+32	-4.18	44351
M1 + P17 → P6 + P36	0.01	1.07E+47	-9.58	29917
	0.1	1.48E+51	-10.63	36022
	1	5.31E+47	-9.49	38643
	2.5	1.28E+43	-8.11	37934
	10	4.80E+41	-7.57	41809
	100	7.91E+39	-6.79	51714
M1 + P17 → M41	0.01	4.76E+68	-17.25	26292
	0.1	9.15E+51	-12.17	18071
	1	9.18E+32	-6.58	6260
	2.5	5.44E+32	-6.47	5802
	10	2.88E+39	-8.30	9788
	100	1.09E+60	-13.93	23557
M1 + P17 → M42	0.01	2.33E+68	-16.69	25474
	0.1	9.96E+60	-14.22	24242
	1	2.28E+51	-11.16	21670
	2.5	6.26E+48	-10.32	21476
	10	6.08E+44	-8.99	21593
	100	5.60E+37	-6.72	22140
M1 + P17 → M43	0.01	1.17E+72	-17.75	29767
	0.1	3.88E+62	-14.68	27048
	1	1.83E+53	-11.69	24764
	2.5	5.42E+51	-11.14	25267
	10	9.73E+47	-9.89	25627
	100	1.39E+41	-7.65	26453
M1 + P17 → M44	0.01	5.30E+58	-14.38	24546
	0.1	2.52E+58	-13.88	27696
	1	1.07E+56	-12.76	31267
	2.5	3.18E+57	-13.02	34452
	10	1.27E+55	-12.07	37352
	100	1.53E+40	-7.38	37071
M1 + P17 → M45	0.01	2.97E+55	-13.40	21399
	0.1	9.84E+56	-13.41	25744
	1	1.13E+55	-12.43	29560
	2.5	5.76E+55	-12.48	32226
	10	5.12E+54	-11.91	36035
	100	4.91E+40	-7.48	36344

4.2 Comparison of RRKM/ME Results from the ChemRate and Multiwell Codes for the Thermal Decomposition of 2-furanylmethyl and related intermediates

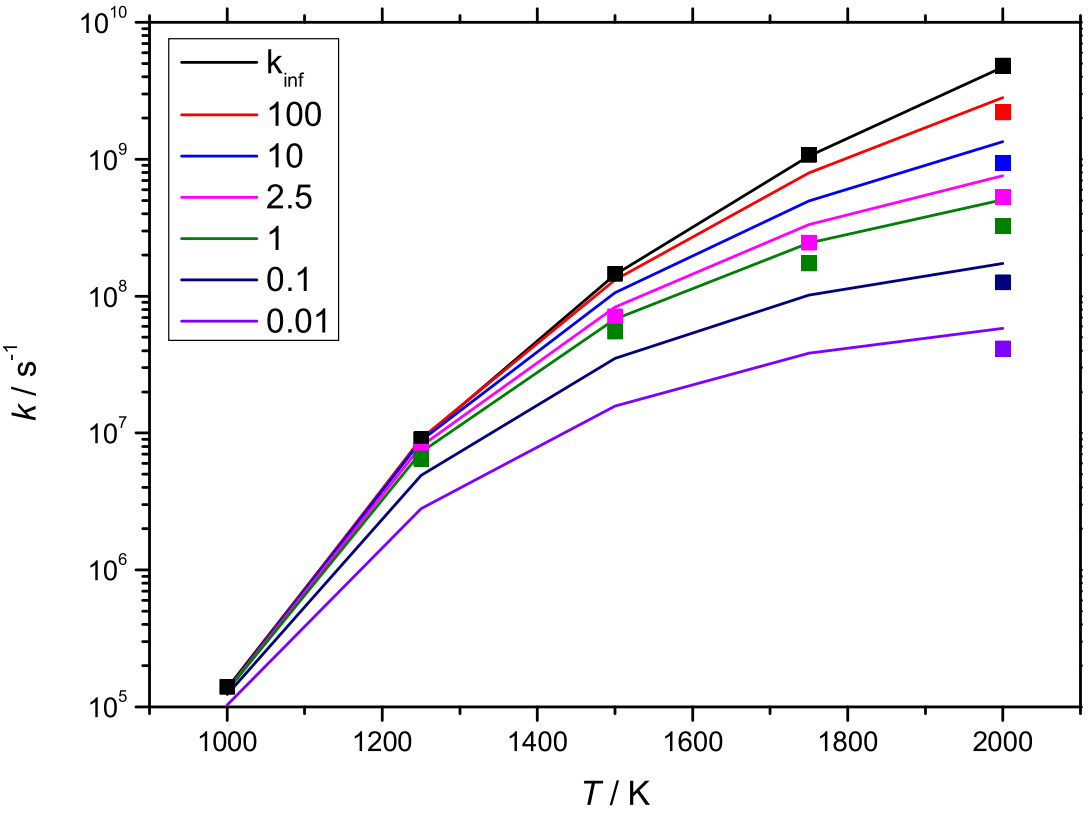

Figure 12: Computed rate constants (p (atm)) for the reaction M10 → M11 from the ChemRate (lines) and Multiwell (symbols) codes.

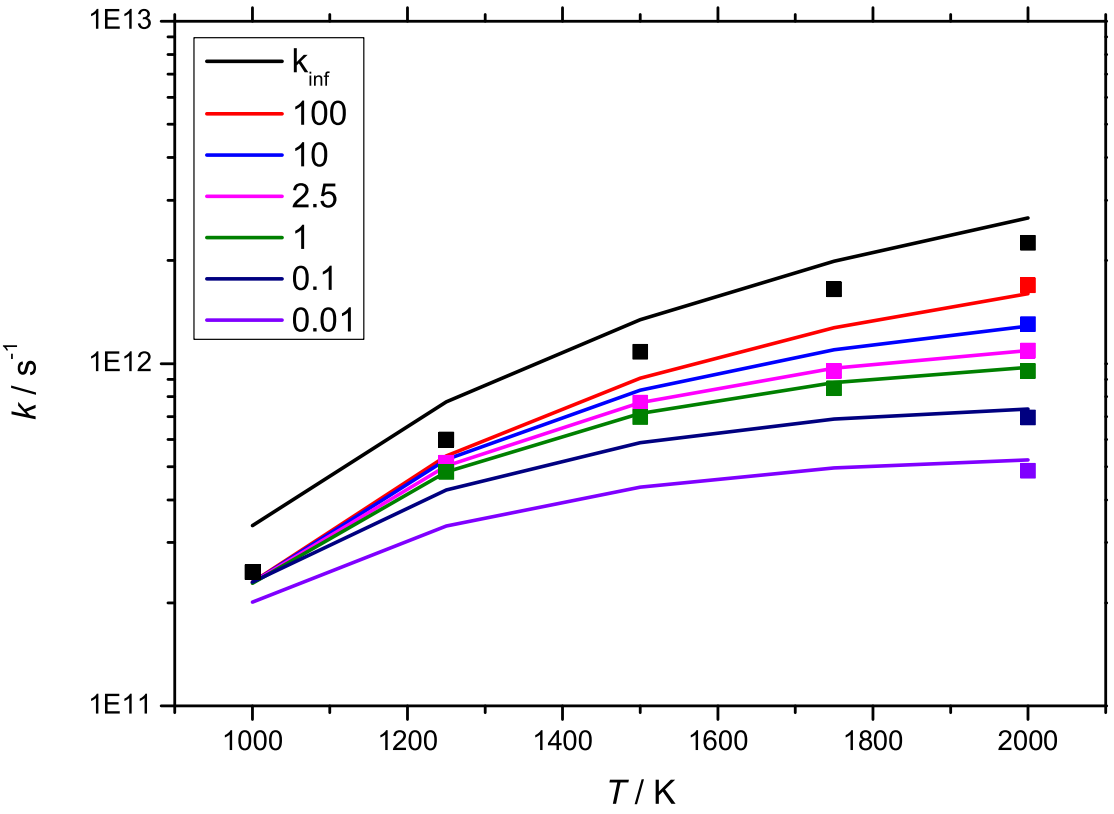

Figure 13: Computed rate constants (p (atm)) for the reaction M11 → M12 from the ChemRate (lines) and Multi-well (symbols) codes.

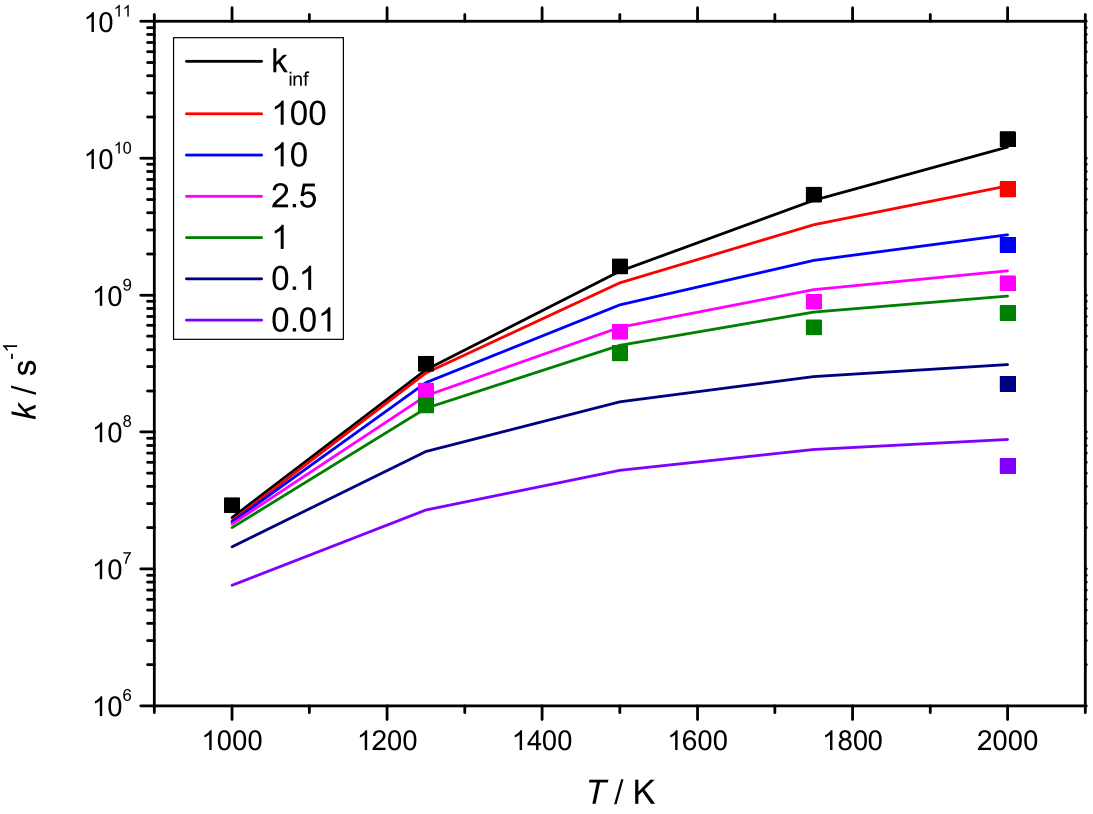

Figure 14: Computed rate constants (p (atm)) for the reaction M12 → M13 from the ChemRate (lines) and Multi-well (symbols) codes.

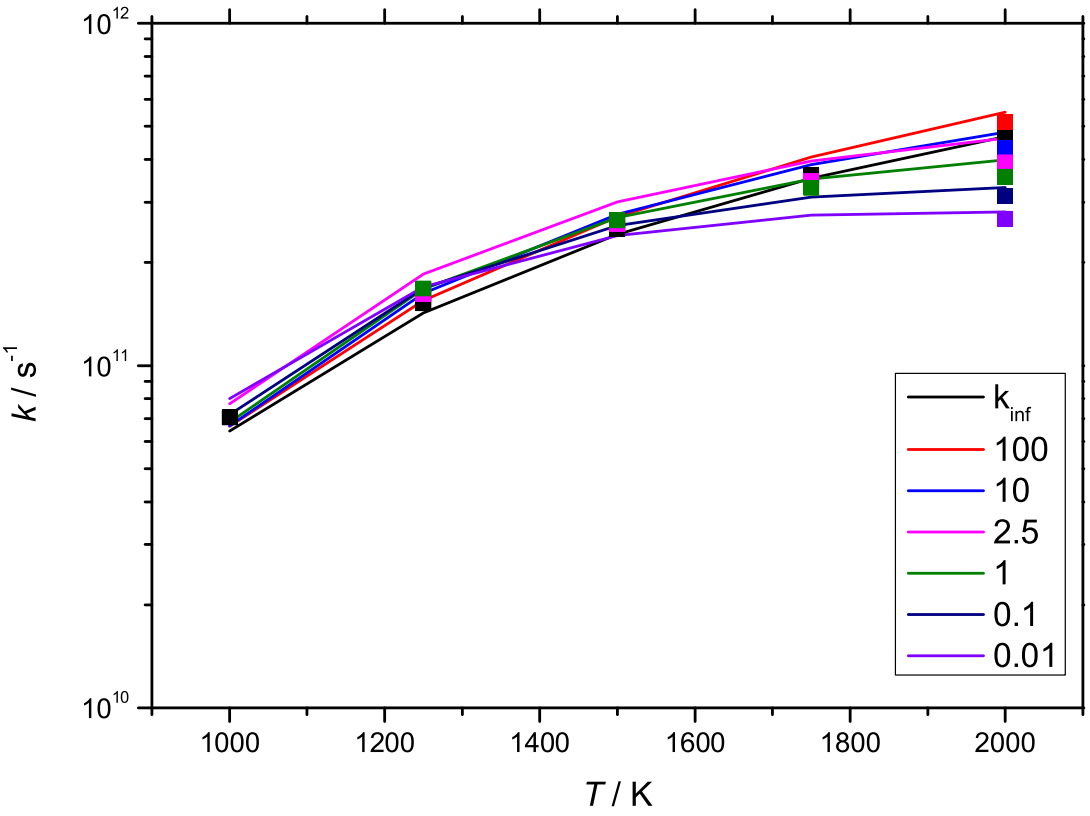

Figure 15: Computed rate constants (p (atm)) for the reaction M13 → M14 from the ChemRate (lines) and Multi-well (symbols) codes.

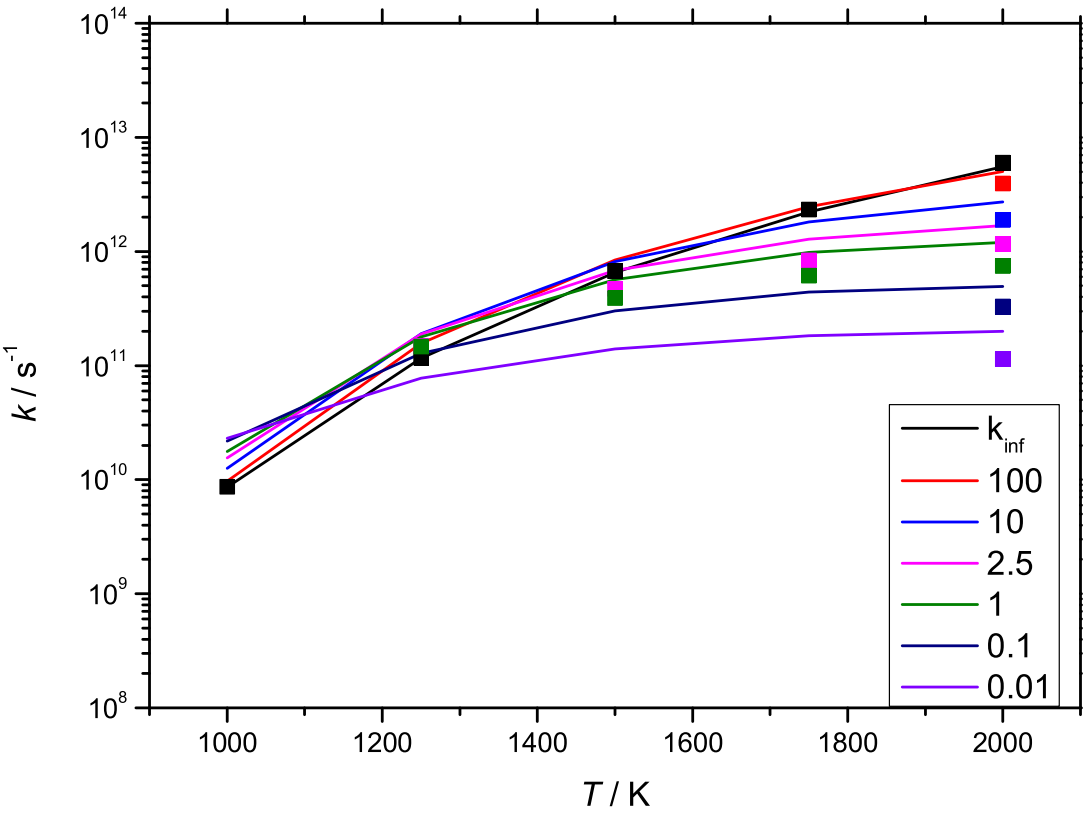

Figure 16: Computed rate constants (p (atm)) for the reaction M14 → P6 + P19 from the ChemRate (lines) and Multiwell (symbols) codes.

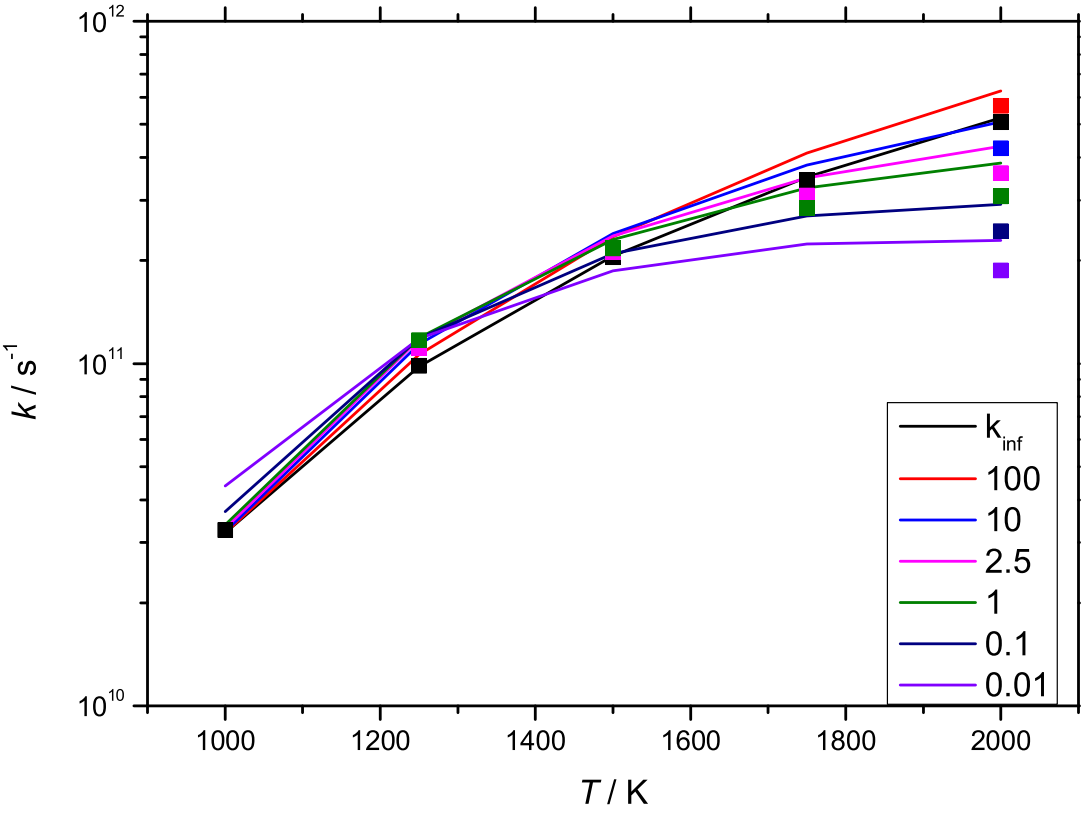

Figure 17: Computed rate constants (p (atm)) for the reaction M13 → M15 from the ChemRate (lines) and Multi-well (symbols) codes.

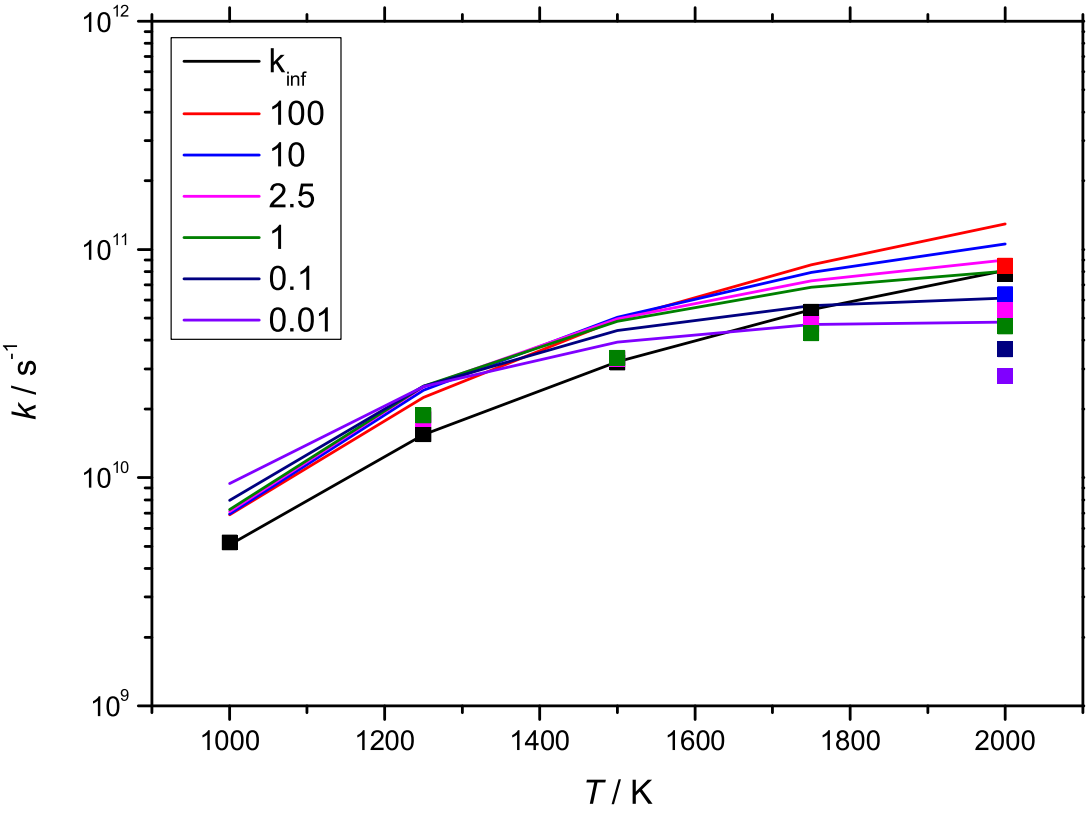

Figure 18: Computed rate constants (p (atm)) for the reaction M15 → M16 from the ChemRate (lines) and Multi-well (symbols) codes.

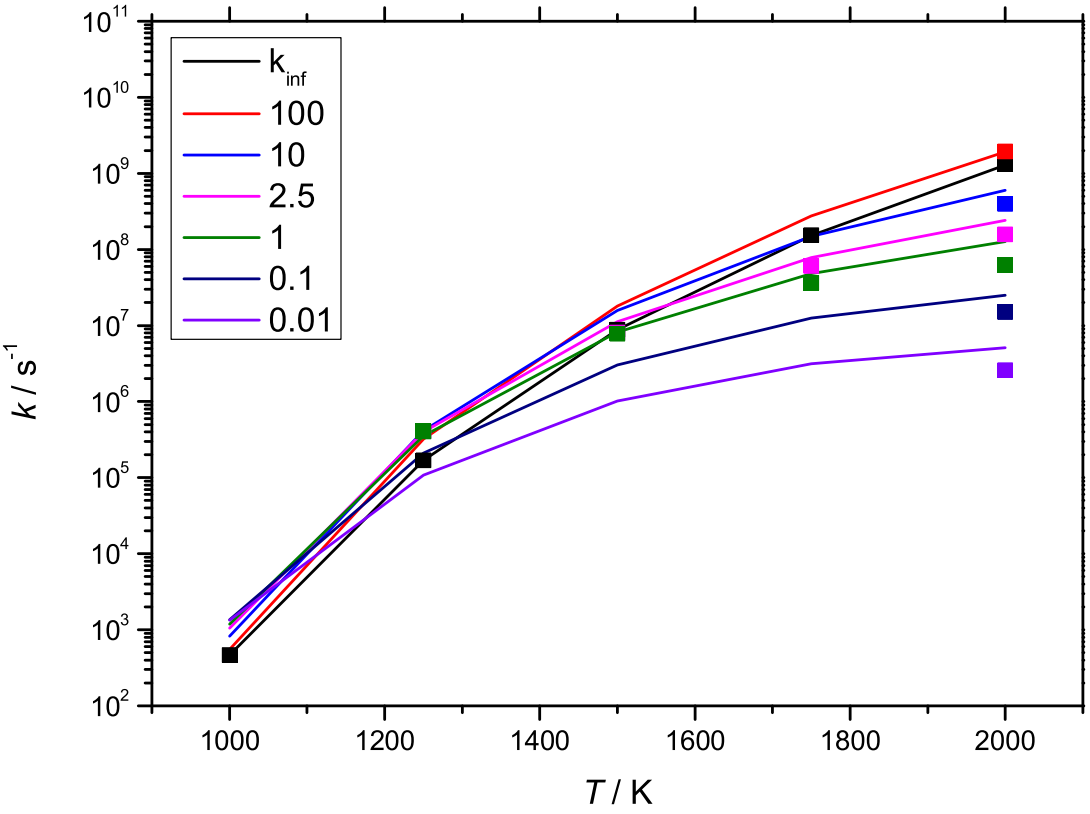

Figure 19: Computed rate constants (p (atm)) for the reaction M16 → P17 + P20 from the ChemRate (lines) and Multiwell (symbols) codes.

5 Comparison of High Pressure Limiting Rate Constants with Literature

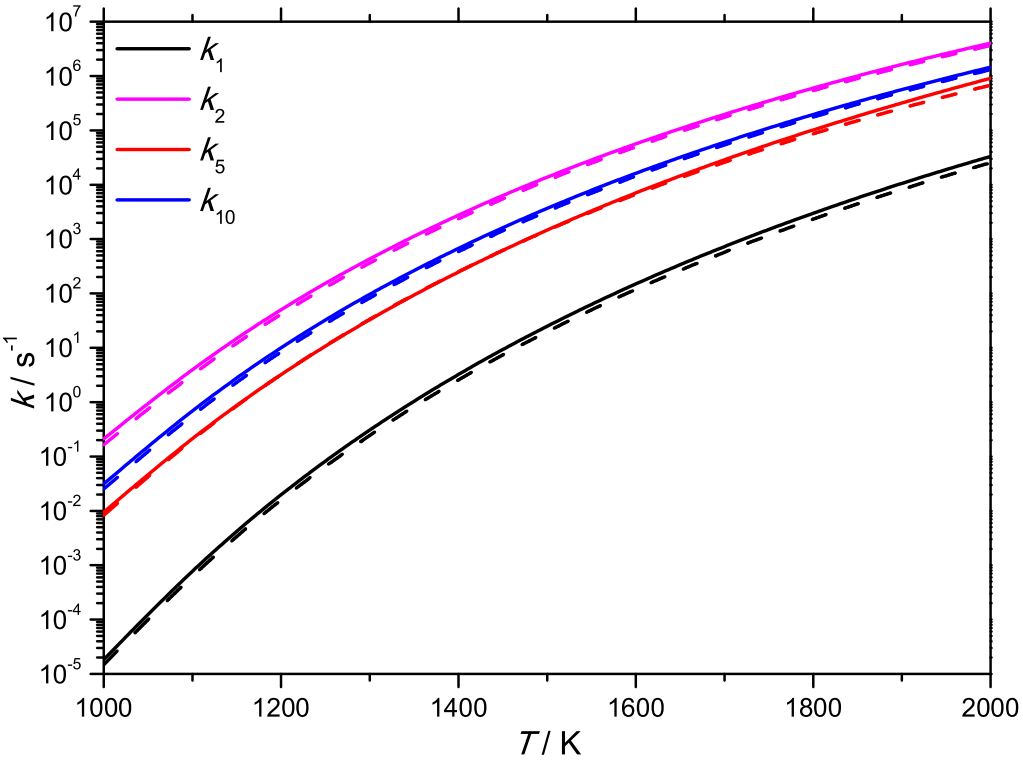

Figure 20: Calculated high-pressure limiting rate constants for hydrogen and methyl group shifts in 2-methylfuran. — Davis and Sarathy [2], – – *this study*. Legend refers to notation in main text. Rate Constants from [2] are multipled by 2 for direct comparison with the results of *this study*, as optical isomer corrections were not accounted for therein.

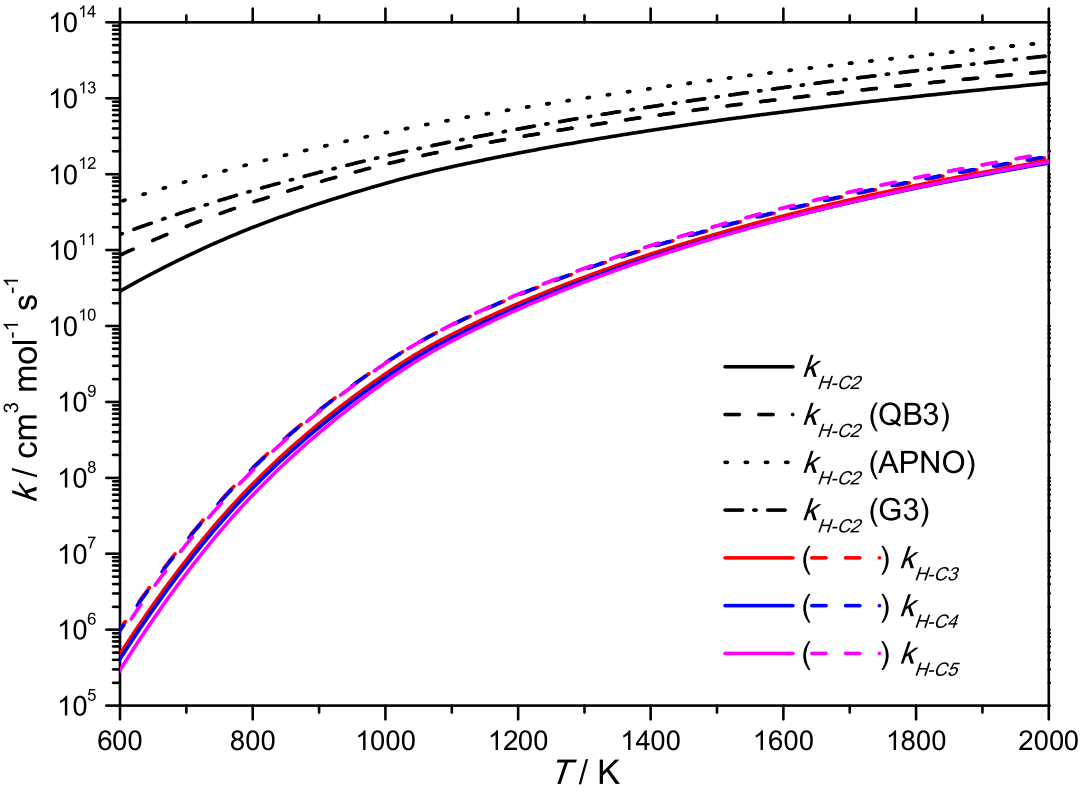

Figure 21: Calculated high pressure limiting rate constants for hydrogen atom abstraction from 2-methylfuran by hydrogen atom. — Davis and Sarathy [2], – – *this study*. Legend refers to notation in main text.

6 Comparison of Mechanism with Literature Oxidation Experiments

6.1 Atmospheric Pressure Ignition Delay Times of 1% 2-Methylfuran/Argon Mixtures

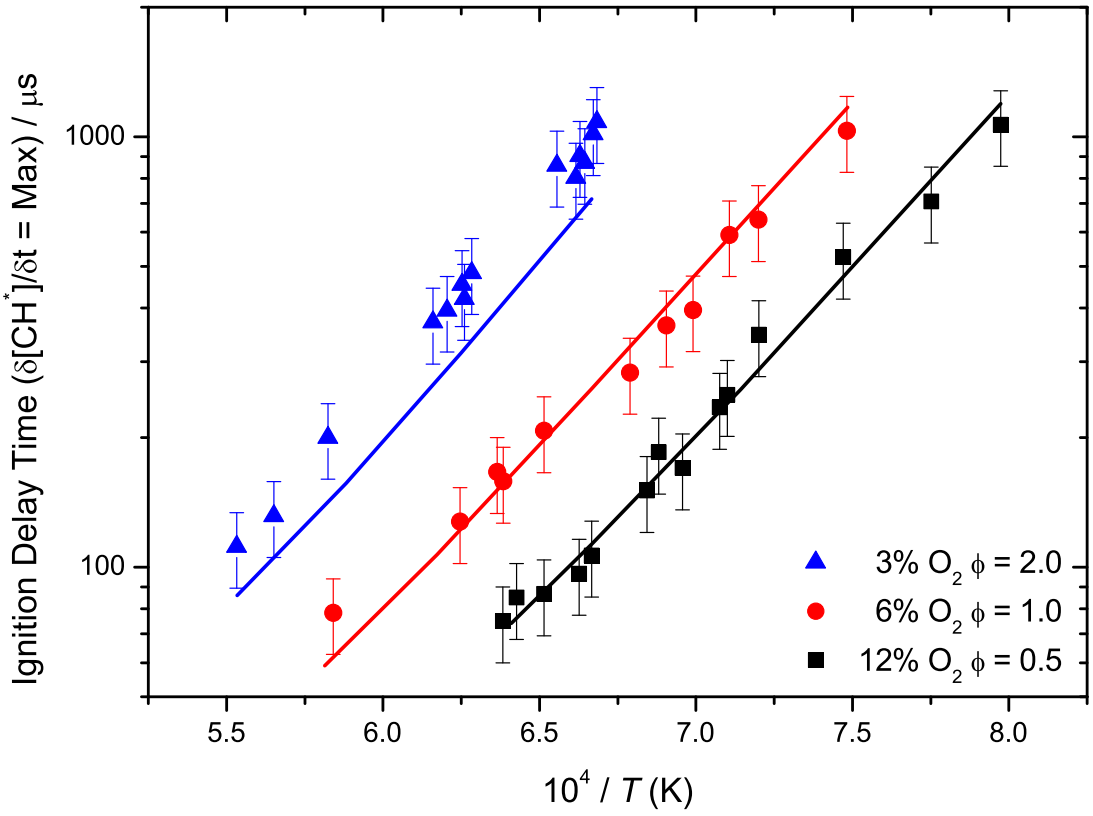

Figure 22: Atmospheric pressures experimental ignition delay times (symbols, [5]) as a function of temperature and O_2 concentration with 20% uncertainty bars and current model predictions (lines).

6.2 Ignition Delay Times of 2-Methylfuran/O_2/Argon Mixtures at Elevated Pressures

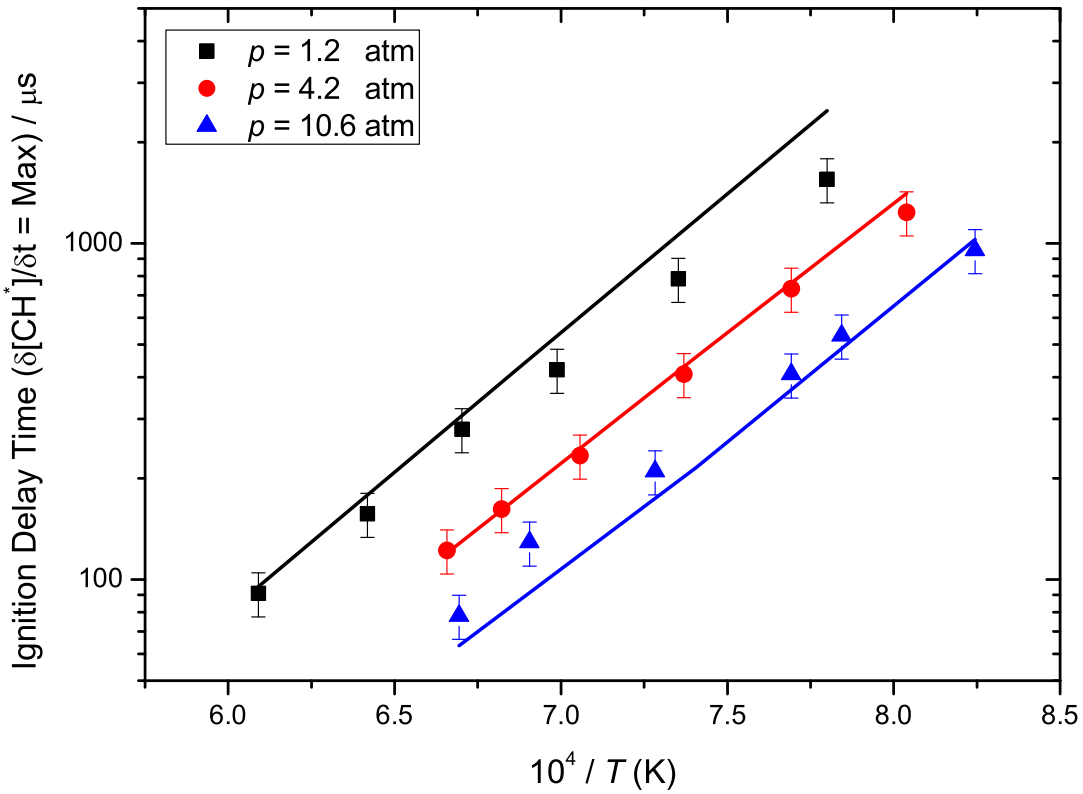

Figure 23: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 0.752% 2MF, 4.511% O_2 and 94.737% Ar (ϕ = 1.0) with modelling calculations (lines).

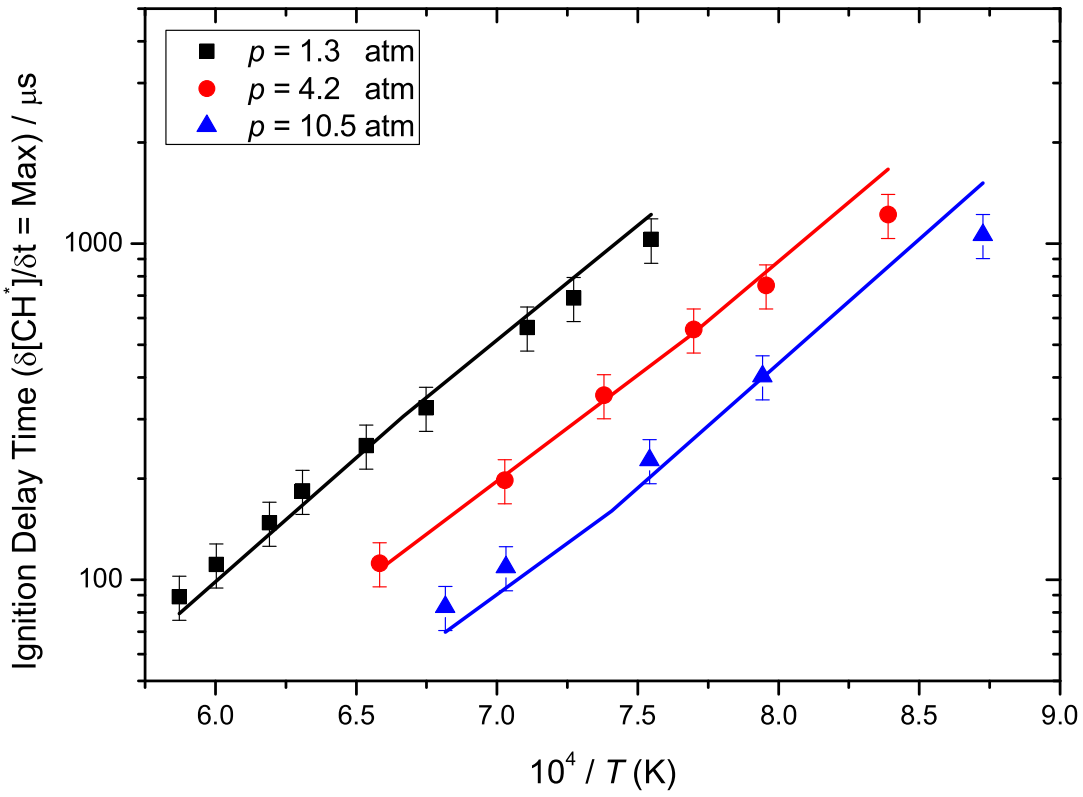

Figure 24: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 1.98% 2MF, 5.941% O_2 and 92.079% Ar (ϕ = 2.0) with modelling calculations (lines).

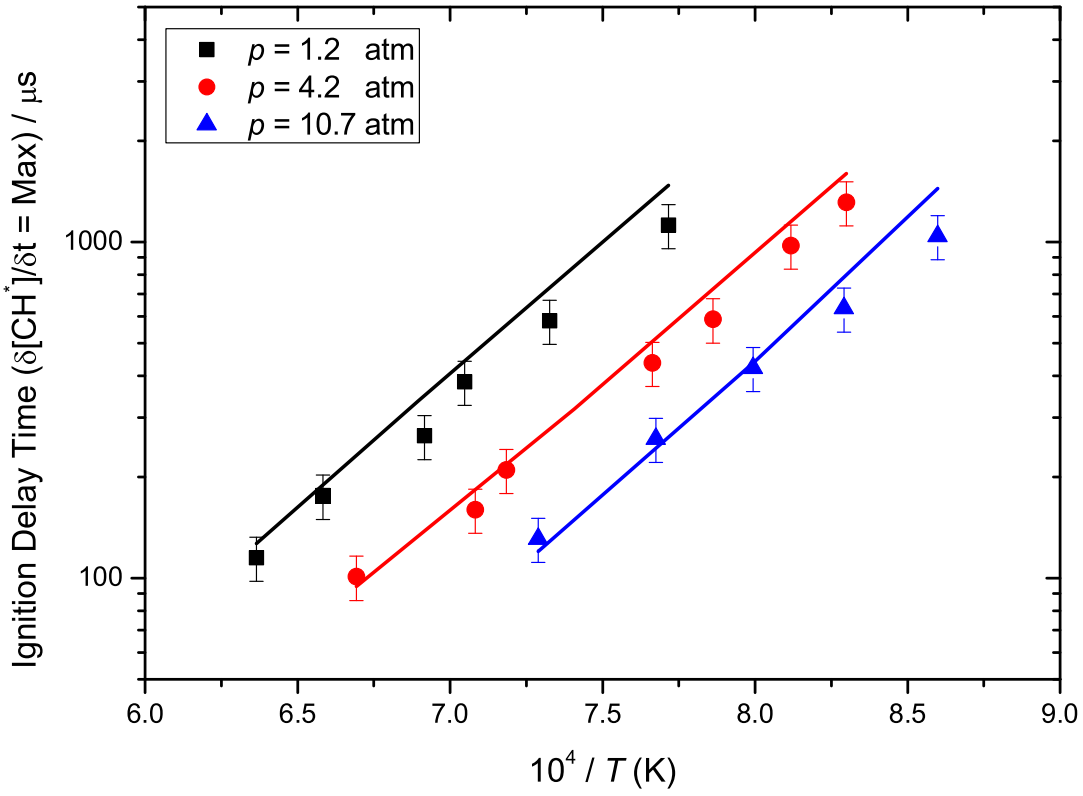

Figure 25: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 1.0% 2MF, 6.0% O_2 and 93.0% Ar (ϕ = 1.0) with modelling calculations (lines).

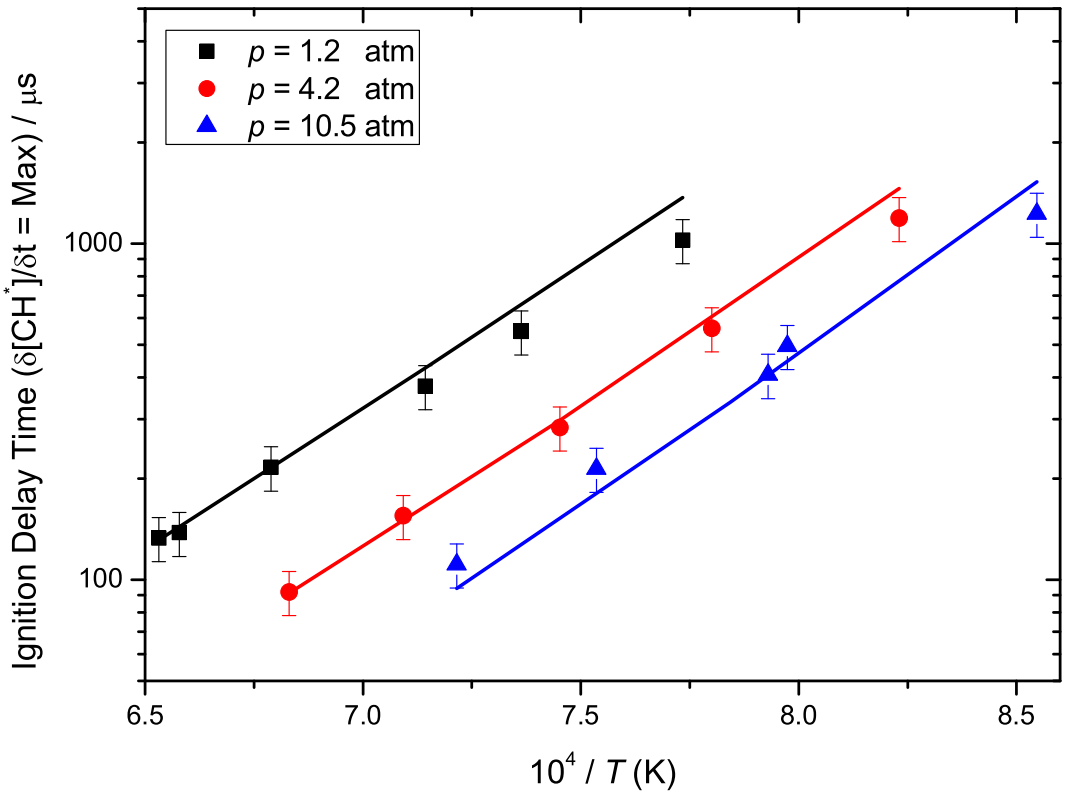

Figure 26: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 0.503% 2MF, 6.030% O_2 and 93.467% Ar (ϕ = 0.5) with modelling calculations (lines).

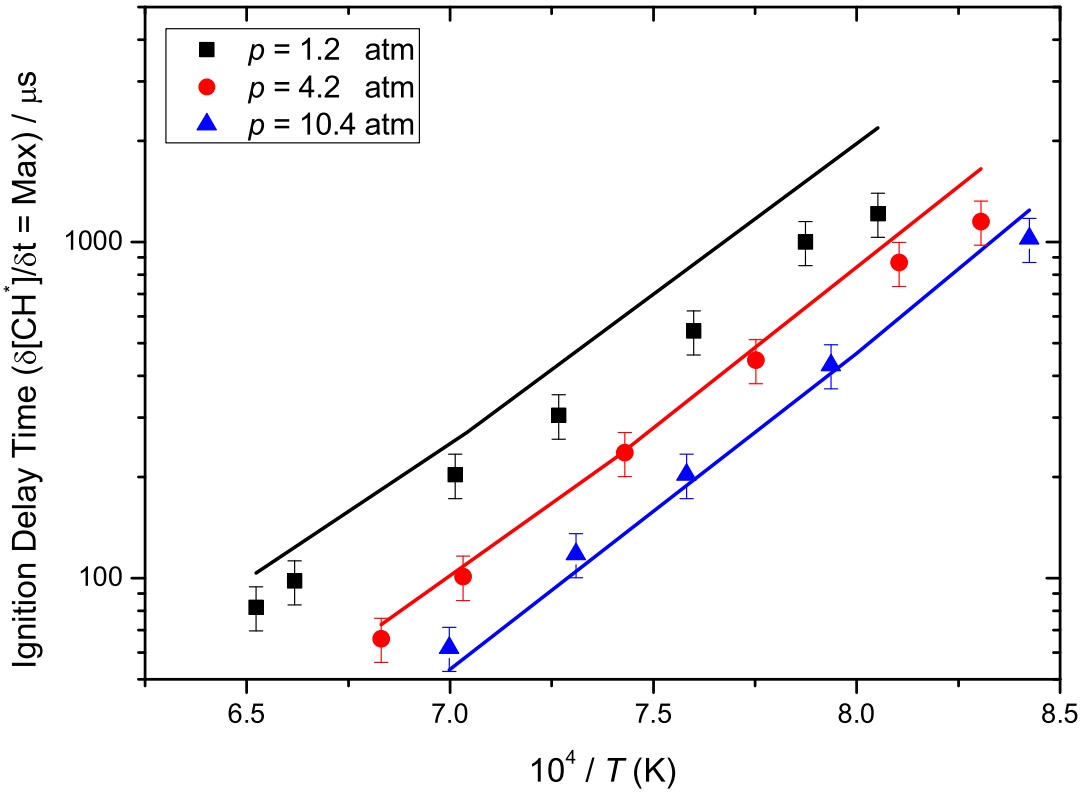

Figure 27: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 0.252% 2MF, 6.045% O_2 and 93.703% (ϕ = 0.25) Ar with modelling calculations (lines).

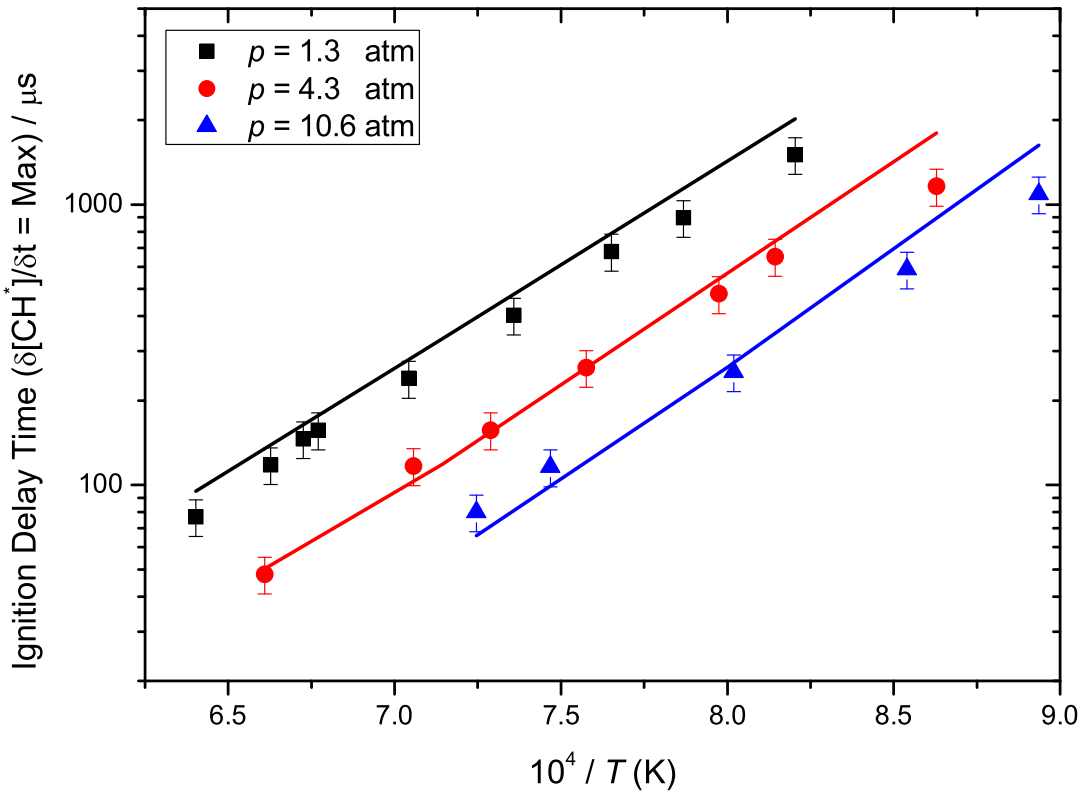

Figure 28: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 1.506% 2MF, 9.036% O_2 and 89.448% Ar (ϕ = 1.0) with modelling calculations (lines).

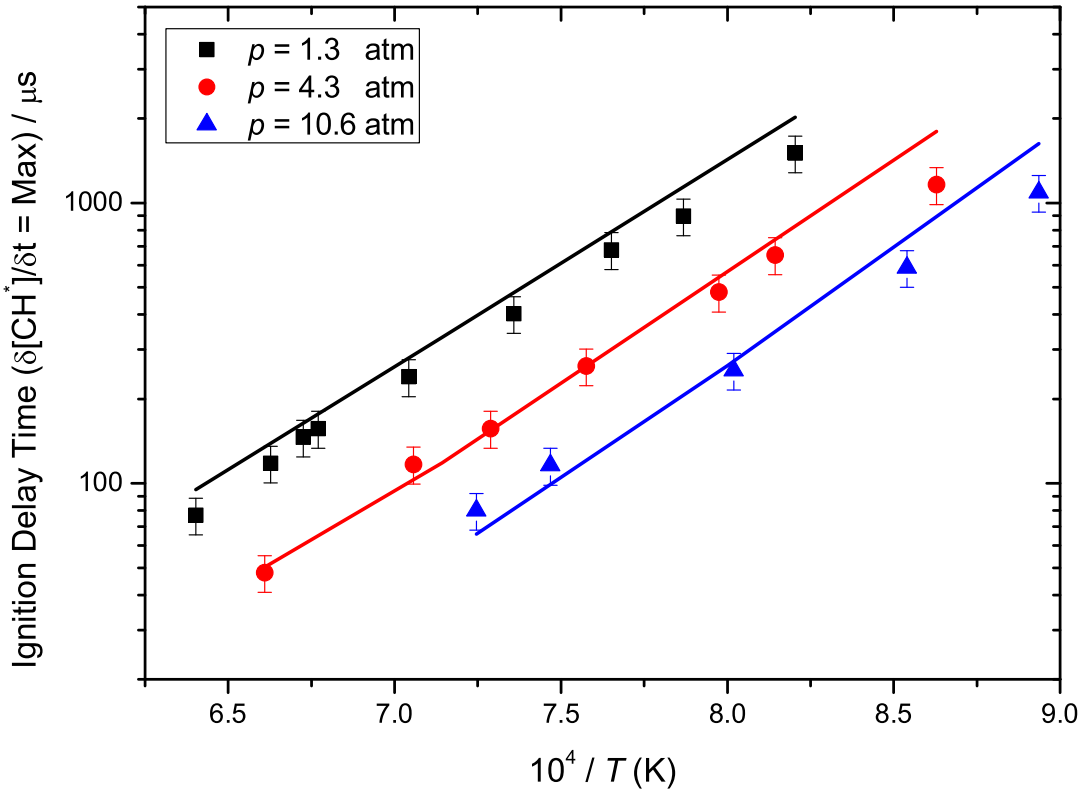

Figure 29: Experimental ignition delay times with 15% uncertainty bars (symbols, [6]) for 3.383% 2MF, 20.298% O_2 and 76.319% Ar (ϕ = 1.0) with modelling calculations (lines).

6.3 Atmospheric Pressure Laminar Burning Velocities of 2-Methylfuran-Synthetic Air Mixtures

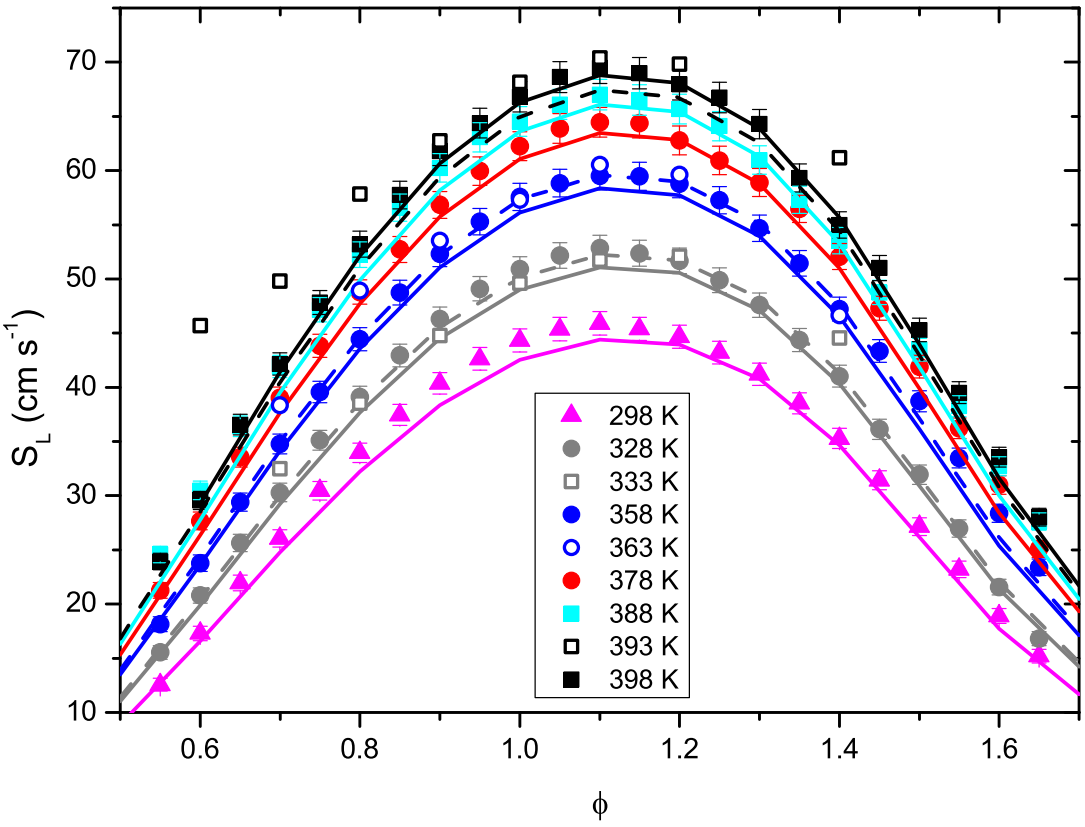

Figure 30: Experimental laminar burning velocities (symbols) as a function of unburnt gas temperature and equivalence ratio with current model predictions (lines). Closed symbols [5] (—) , open symbols [7] (– –).

6.4 Speciation in Low-Pressure 2-Methylfuran/O_2/Ar Flames

6.4.1 ϕ = 1.0

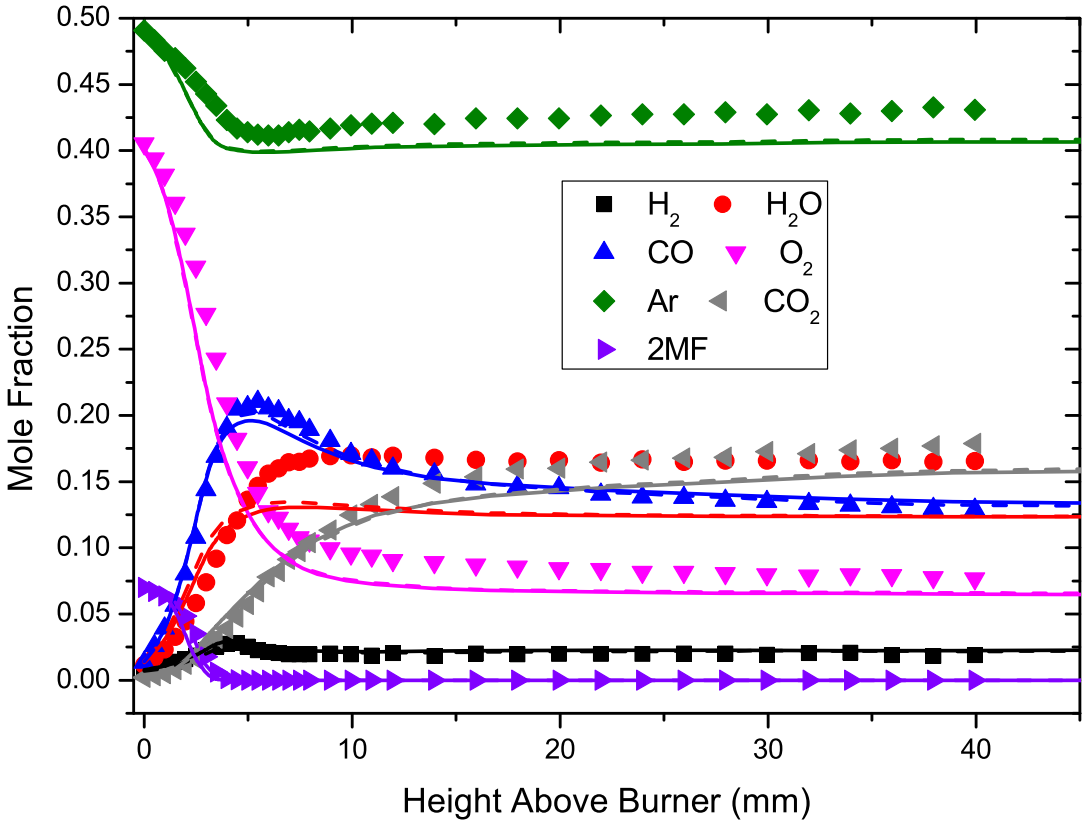

Figure 31: Experimental profiles [8] for main species measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

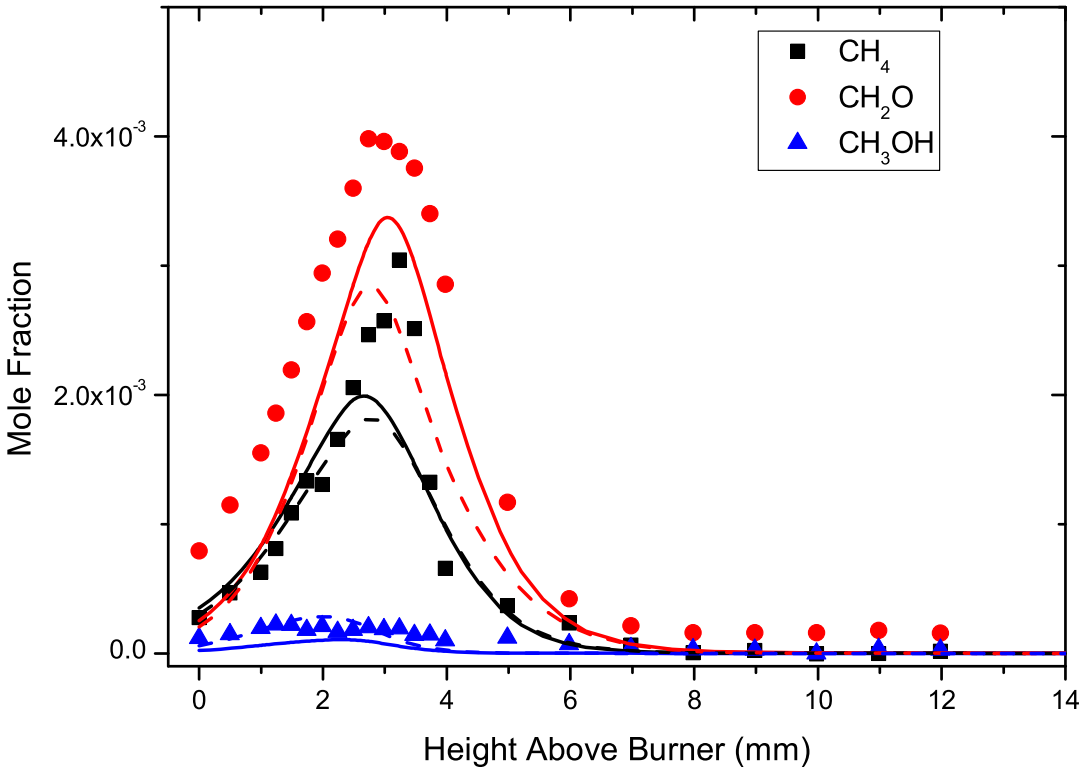

Figure 32: Experimental profiles [8] for methane, formaldehyde and methanol measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

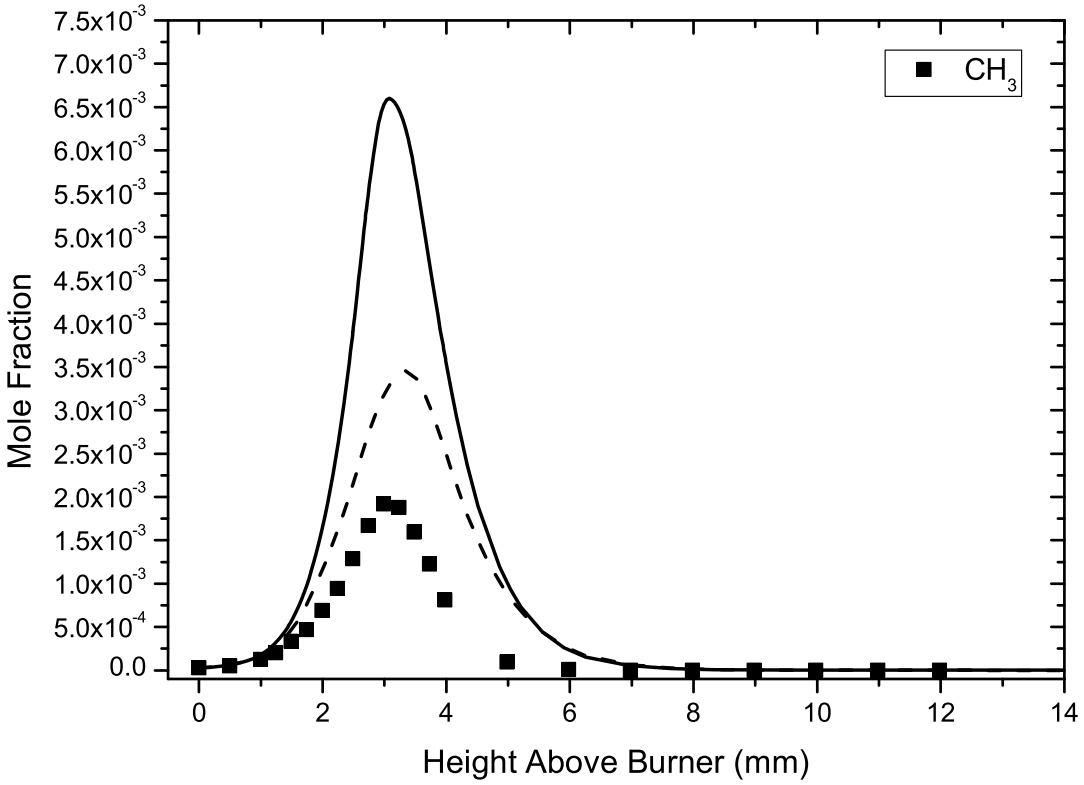

Figure 33: Experimental profile [8] for methyl radical measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –). Refer to [8] for a discussion on the uncertainties (up to a factor of 4) in the determination of concentrations of small radicals.

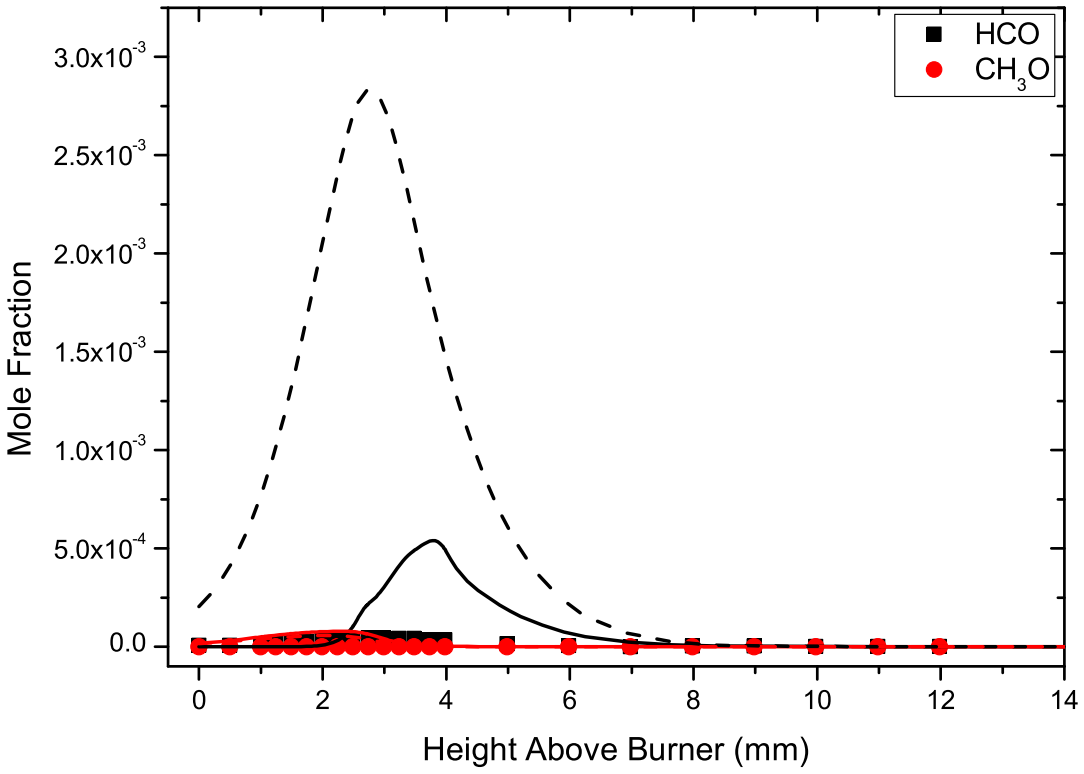

Figure 34: Experimental profiles [8] for formyl and methoxy radicals measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

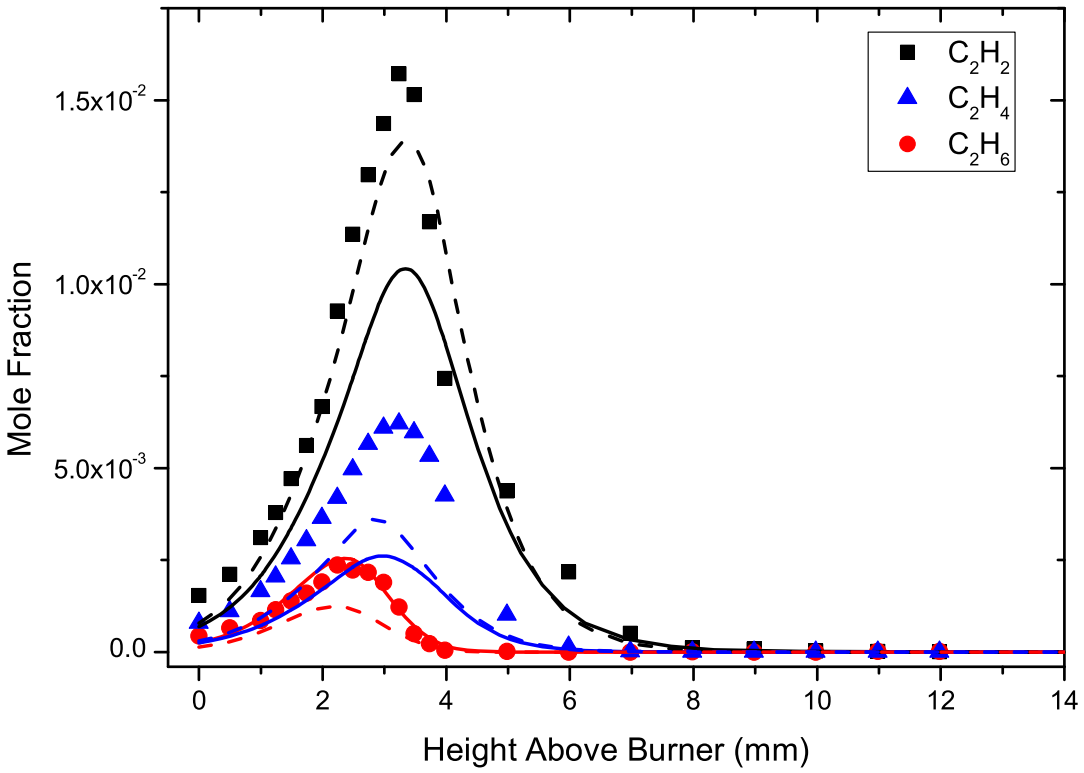

Figure 35: Experimental profiles [8] for acetylene, ethylene and ethane measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

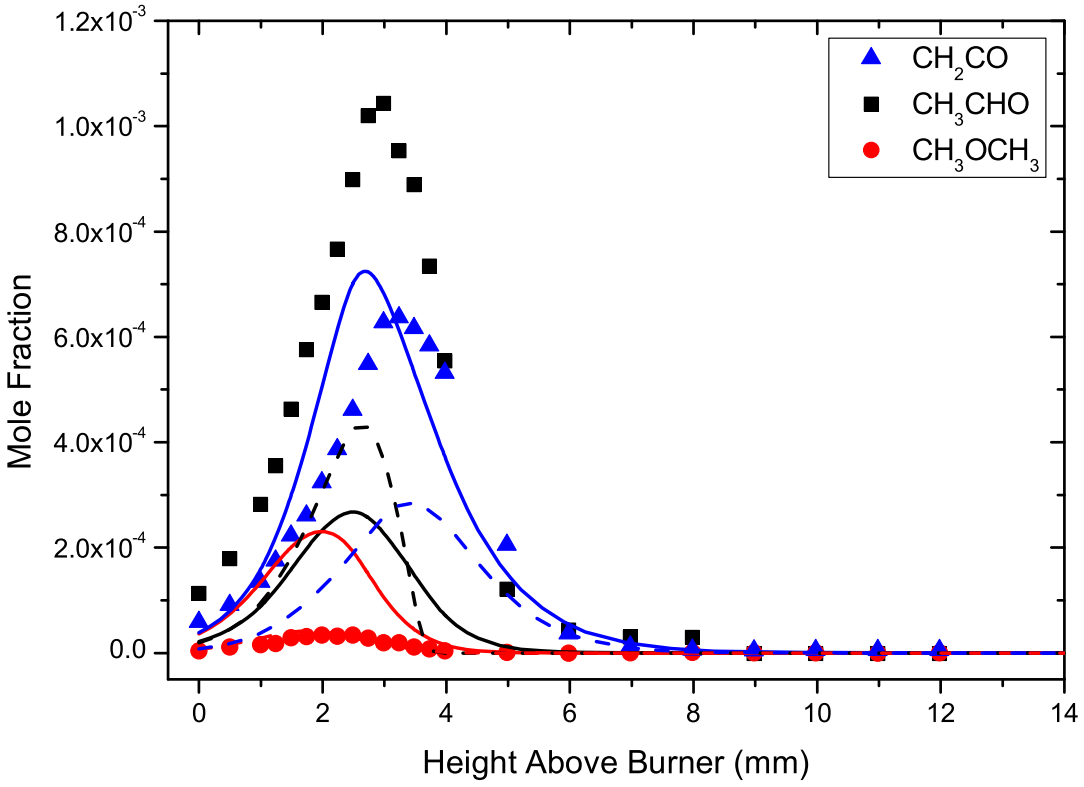

Figure 36: Experimental profiles [8] for ketene, acetaldehyde and dimethyl ether measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

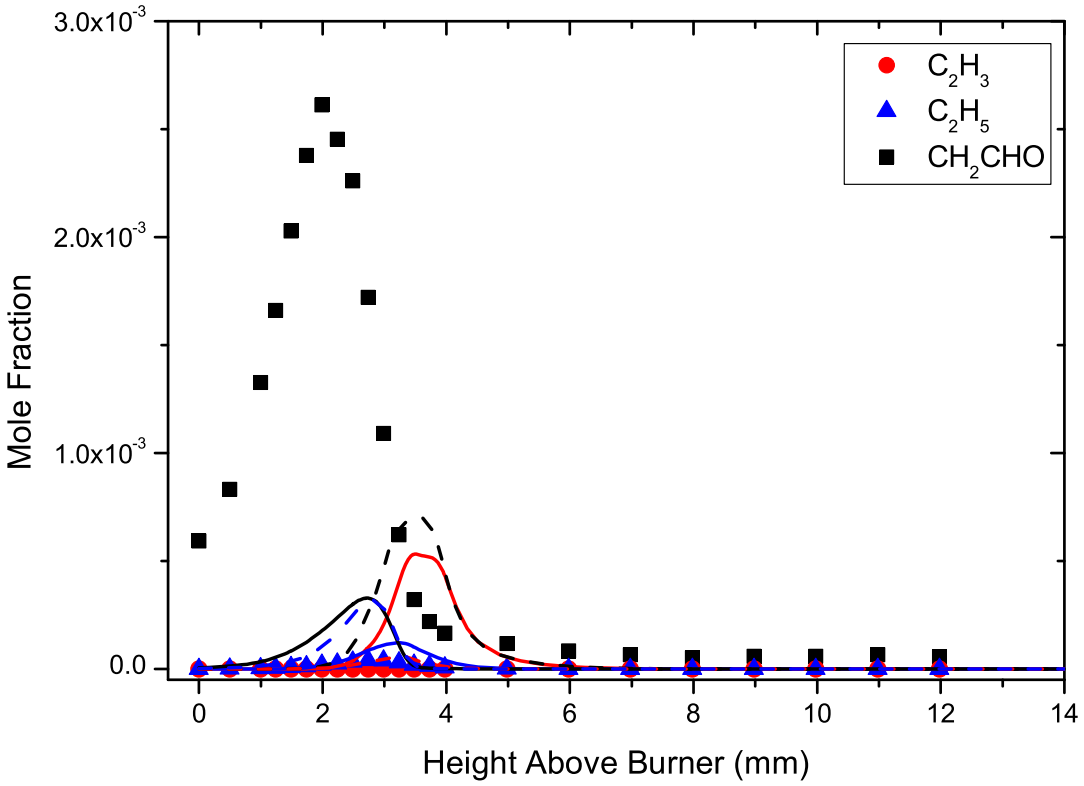

Figure 37: Experimental profiles [8] for vinyl, ethyl and vinoxy radicals measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

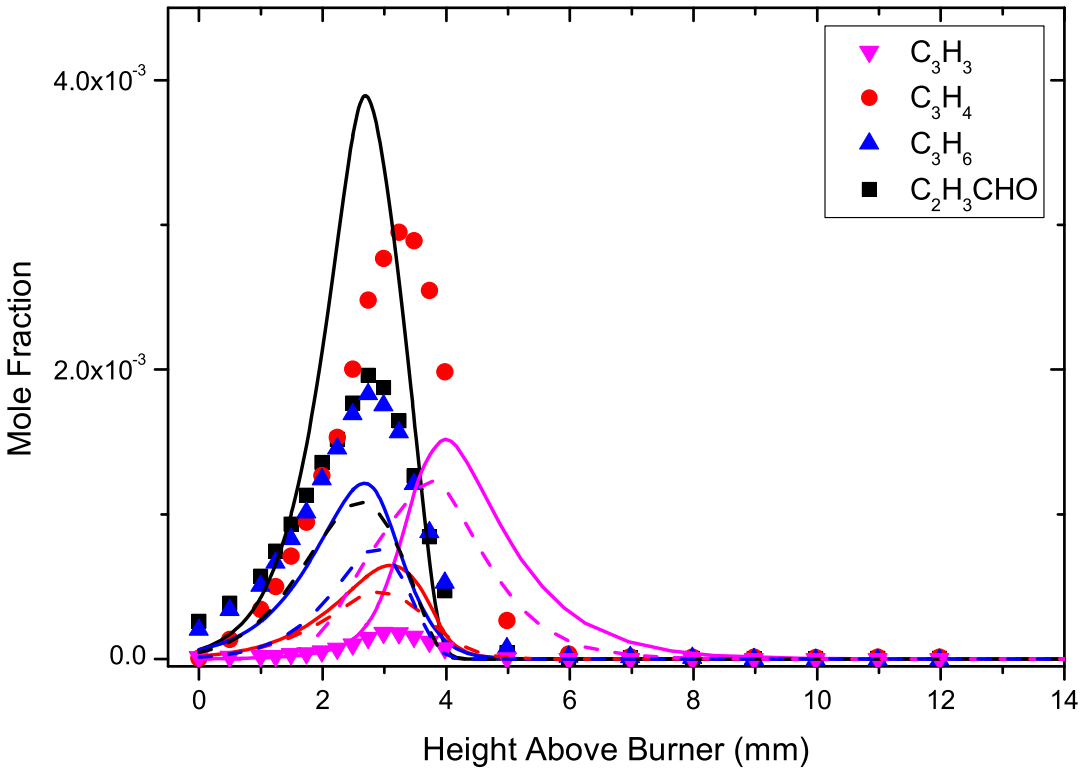

Figure 38: Experimental profiles [8] for propargyl radical, propyne, propene and acrolein measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

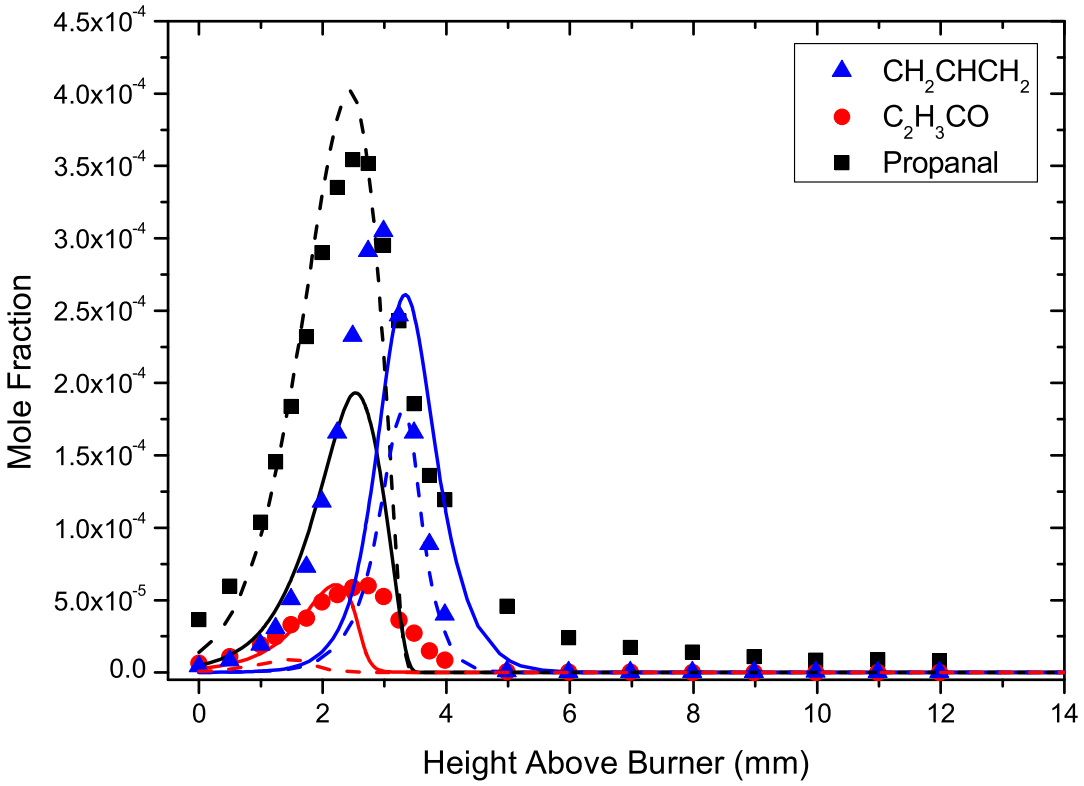

Figure 39: Experimental profiles [8] for allyl and acrolein radicals and propanal measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

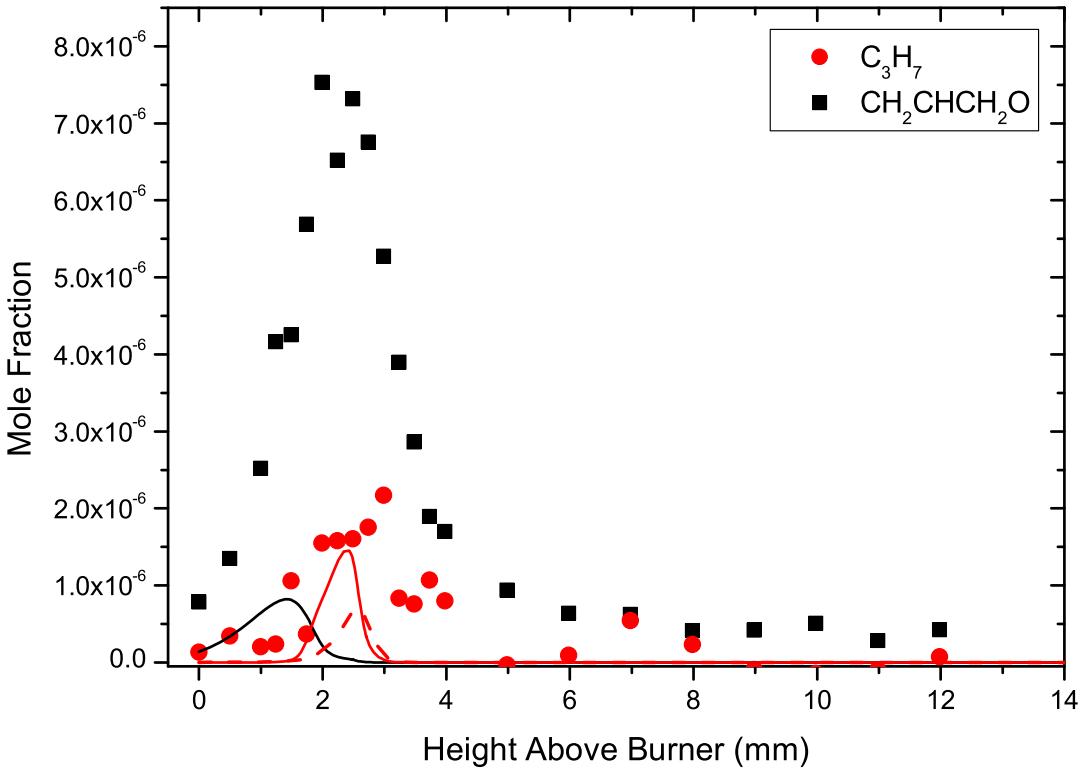

Figure 40: Experimental profiles [8] for *n*-propyl and allyloxy radicals measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

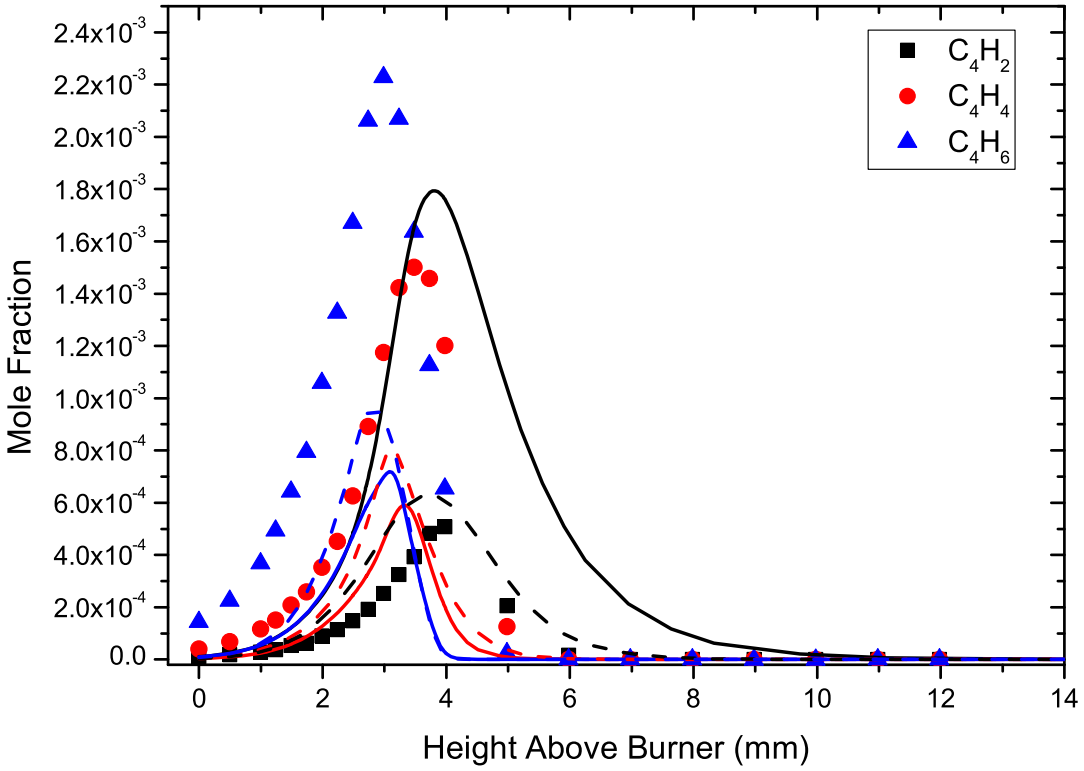

Figure 41: Experimental profiles [8] for diacetylene, vinylacetylene and 1,3-butadiene measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

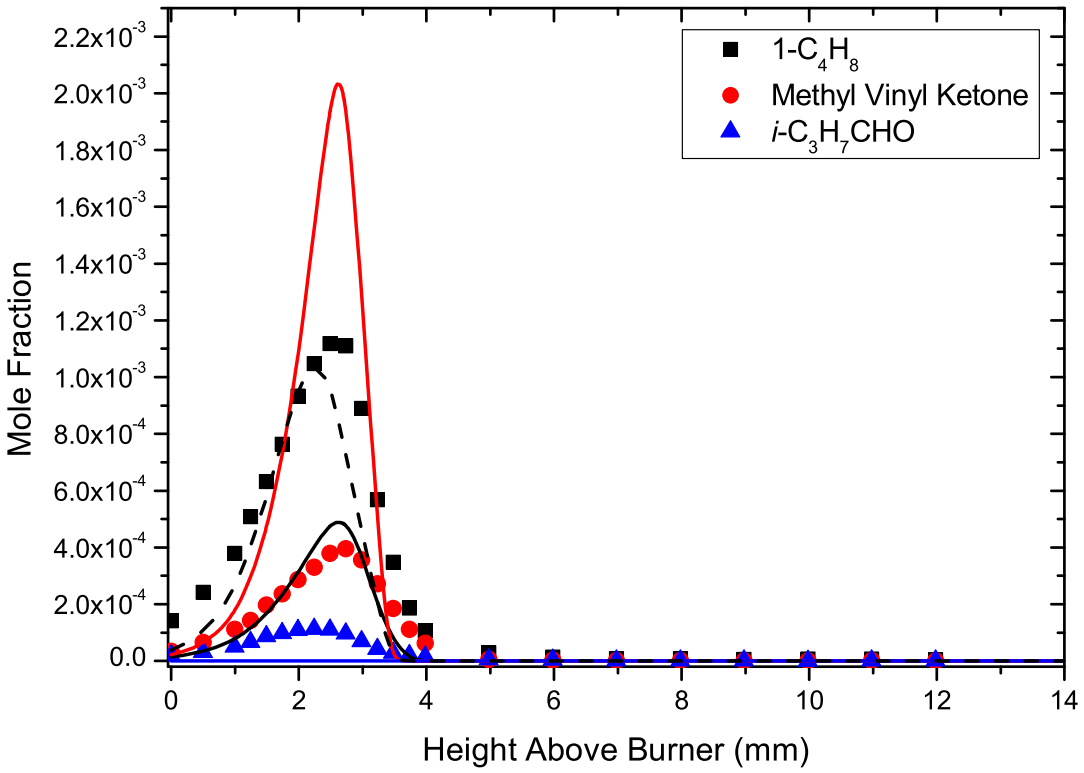

Figure 42: Experimental profiles [8] for 1-butene, methyl vinyl ketone and *butanal* measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

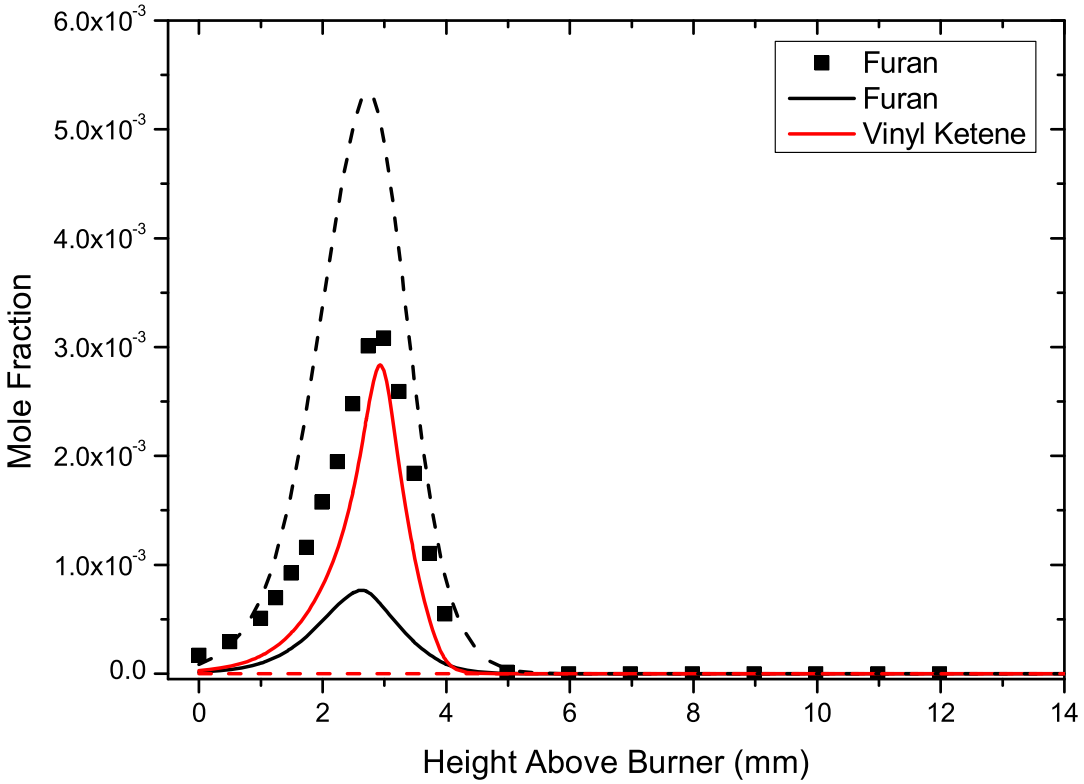

Figure 43: Experimental profiles [8] for furan measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –). Vinyl ketene yields, which were not quantified experimentally, are included for comparison.

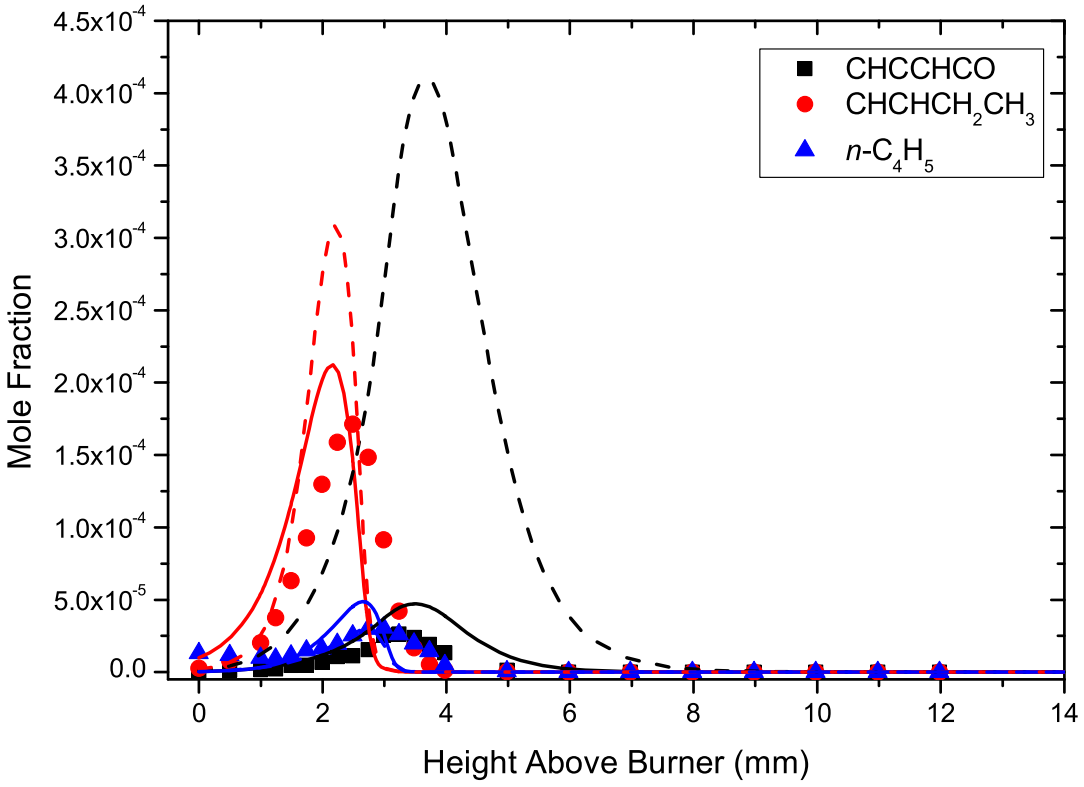

Figure 44: Experimental profiles [8] for acetylenylketene, *n*-butenyl and *n*-butadienyl measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

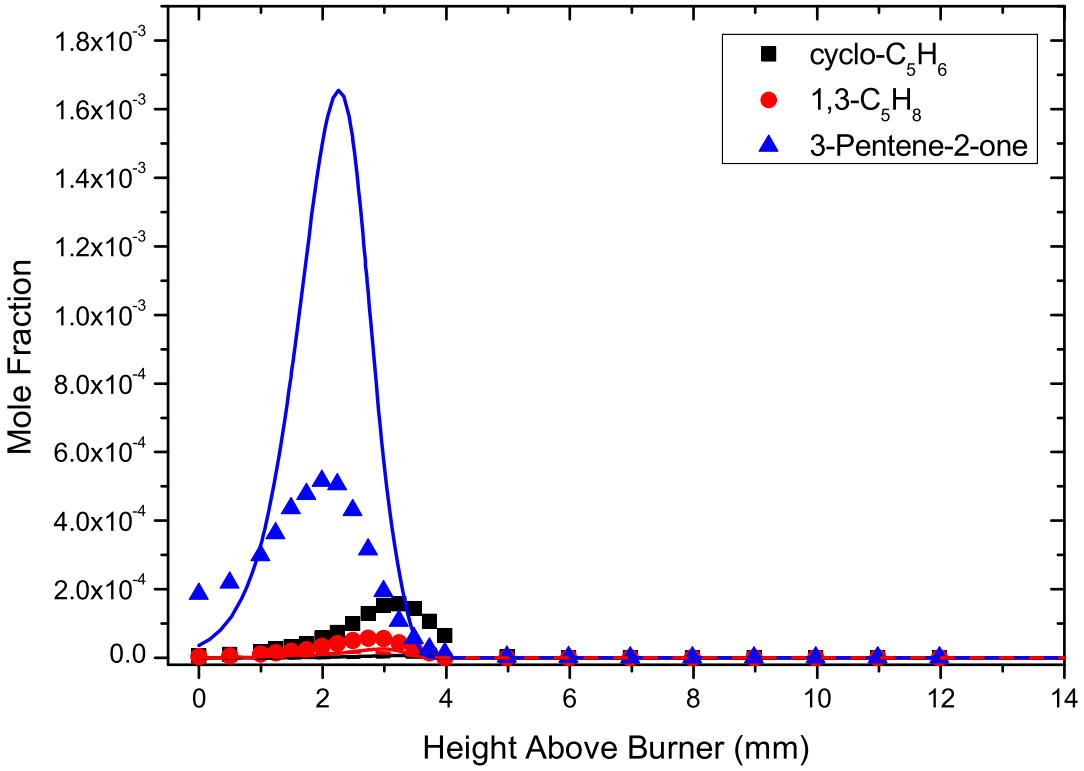

Figure 45: Experimental profiles [8] for 1,3-cyclopentadiene, 1,3-pentadiene and 3-pentene-2-one measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

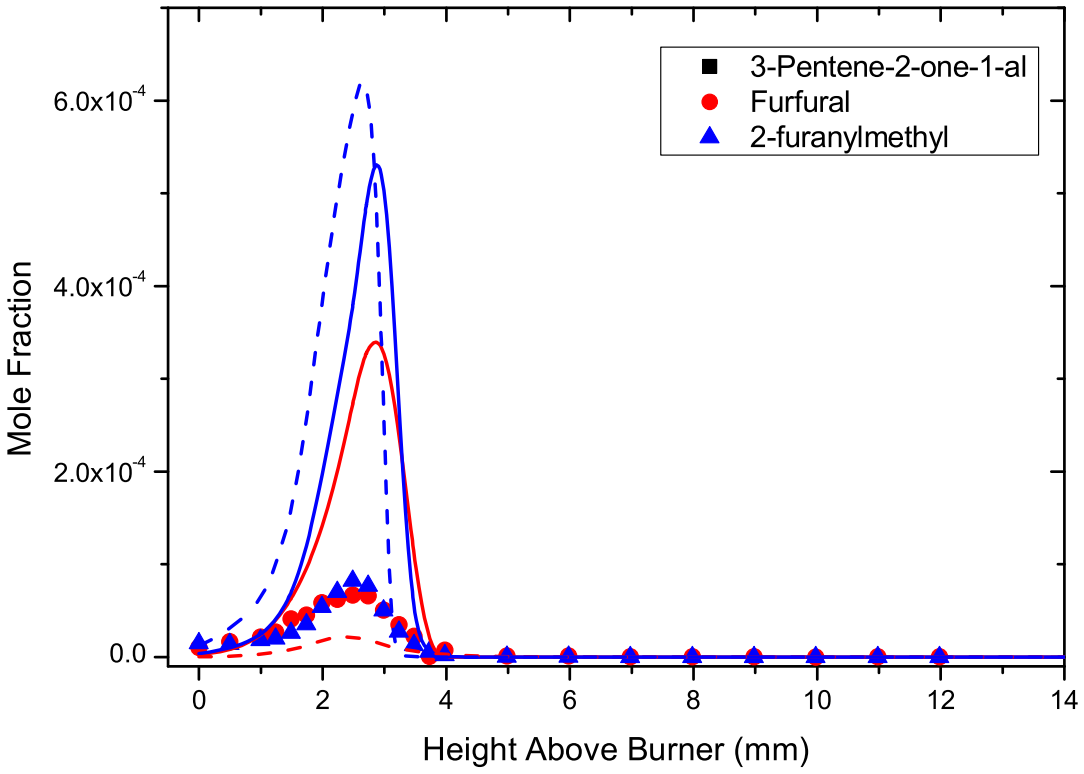

Figure 46: Experimental profiles [8] for 3-pentene-2-one-1-al, furfural and 2-furanylmethyl measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

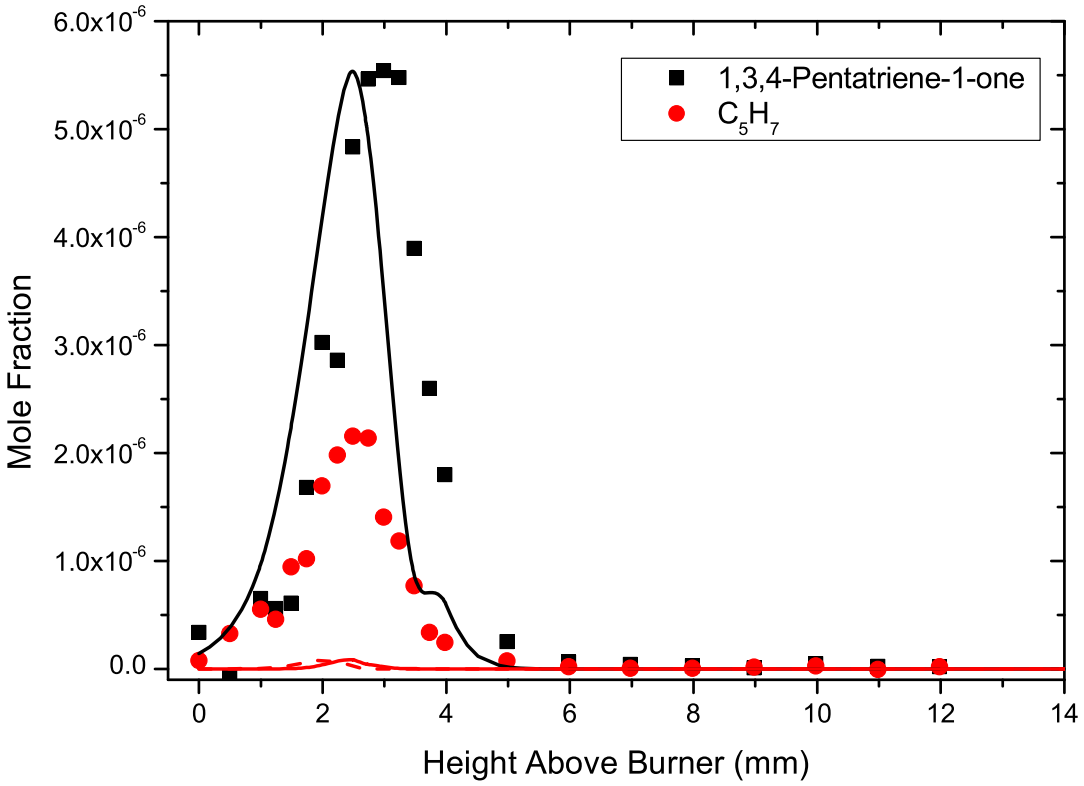

Figure 47: Experimental profiles [8] for 1,3,4-pentatriene-1-one and cyclopenteneyl radical measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

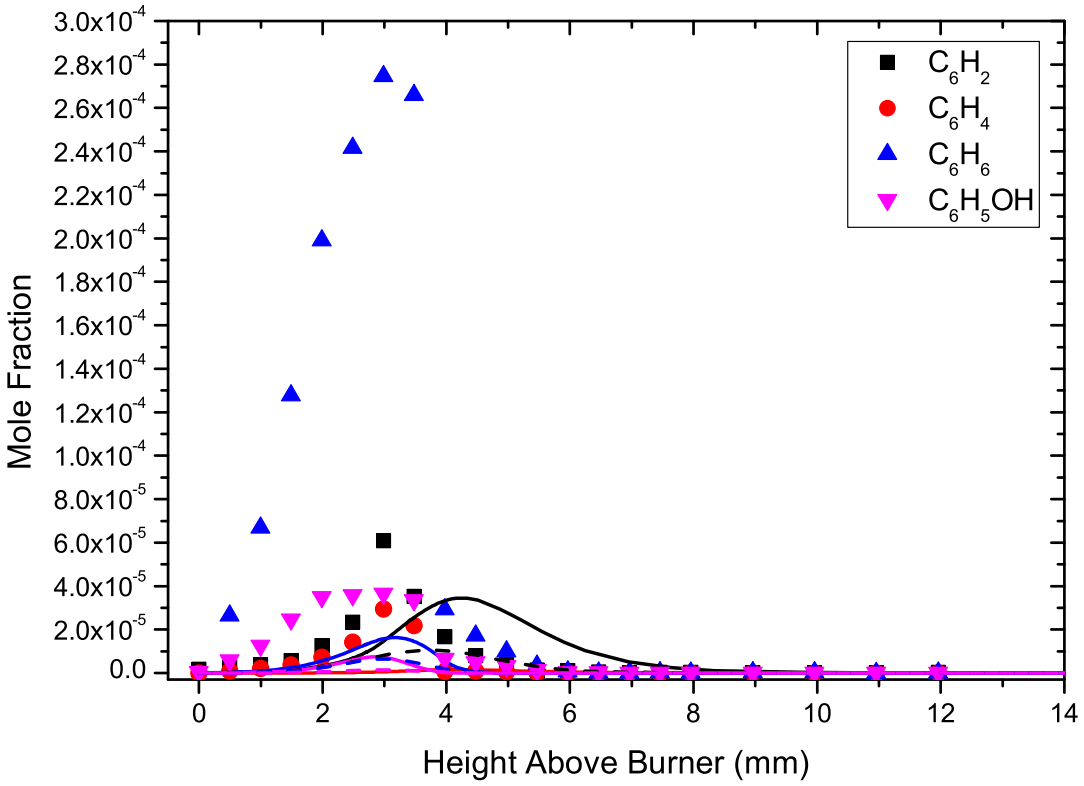

Figure 48: Experimental profiles [8] for triacetylene, benzyne, benzene and phenol measured in ϕ = 1.0 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

6.4.2 ϕ = 1.7

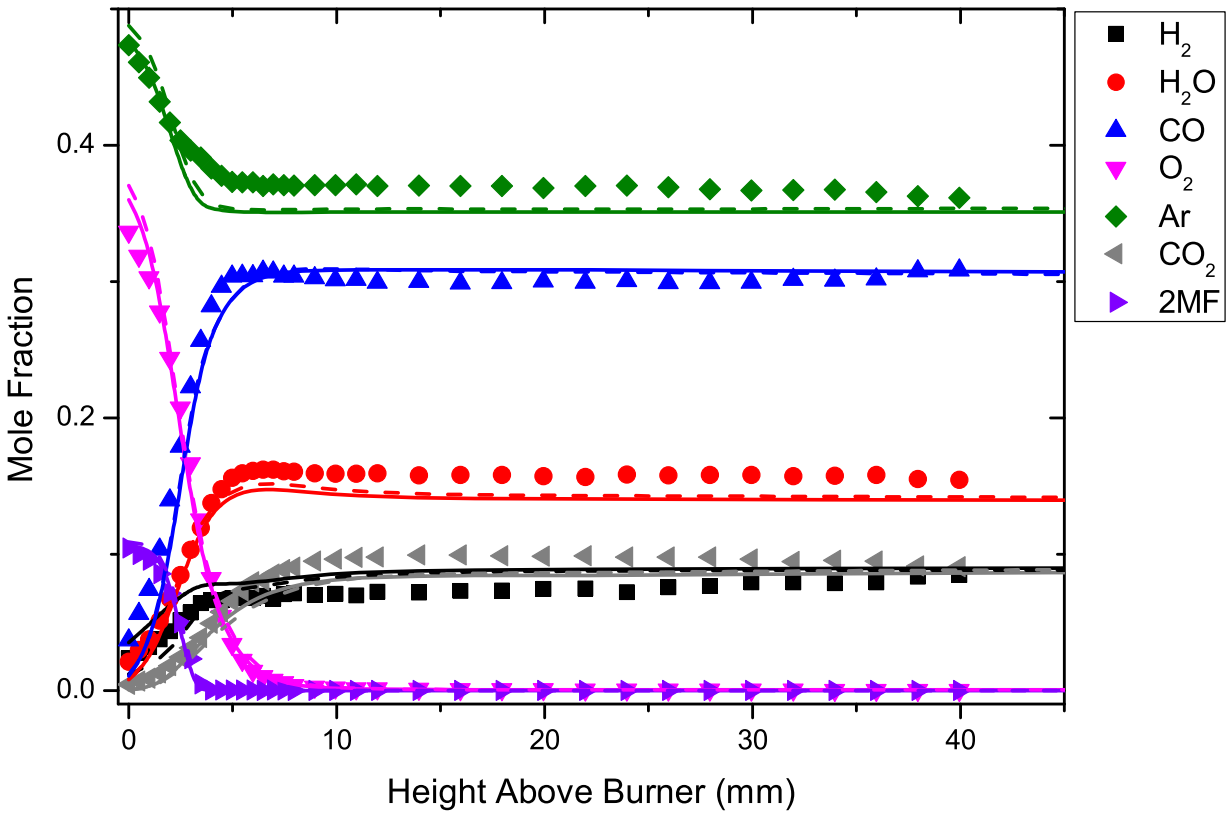

Figure 49: Experimental profiles [8] for main species measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

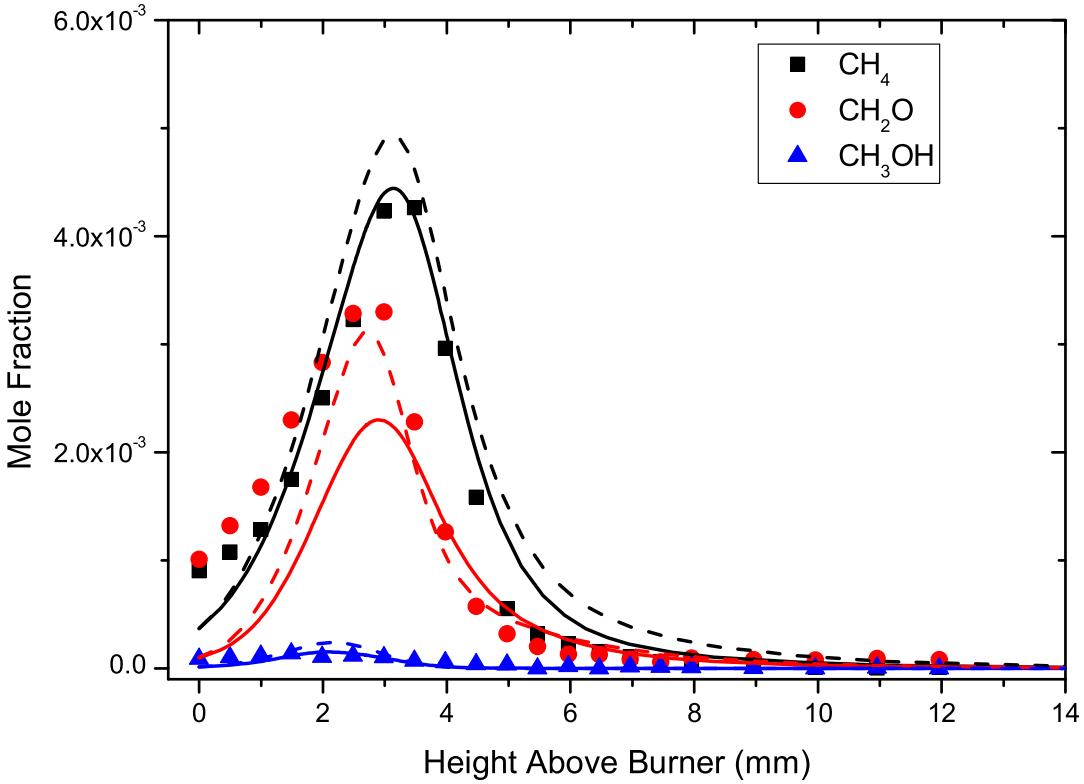

Figure 50: Experimental profiles [8] for methane, formaldehyde and methanol measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

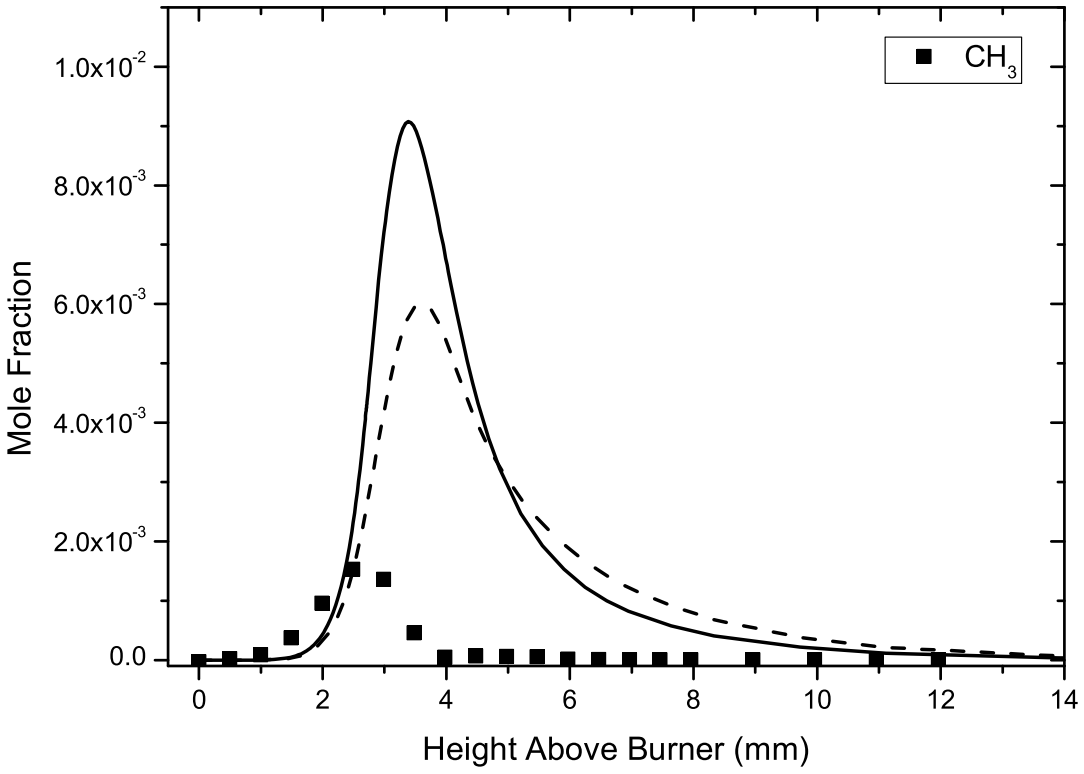

Figure 51: Experimental profile [8] for methyl radical measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –). Refer to [8] for a discussion on the uncertainties (up to a factor of 4) in the determination of concentrations of small radicals.

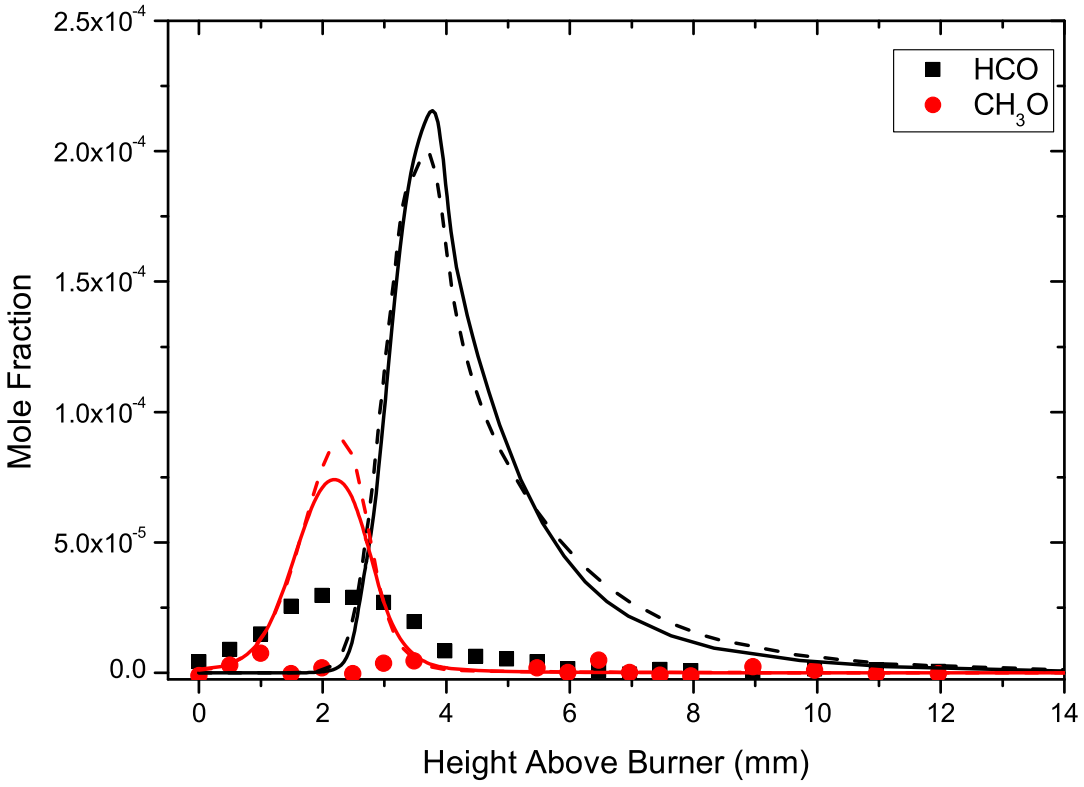

Figure 52: Experimental profiles [8] for formyl and methoxy radicals measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

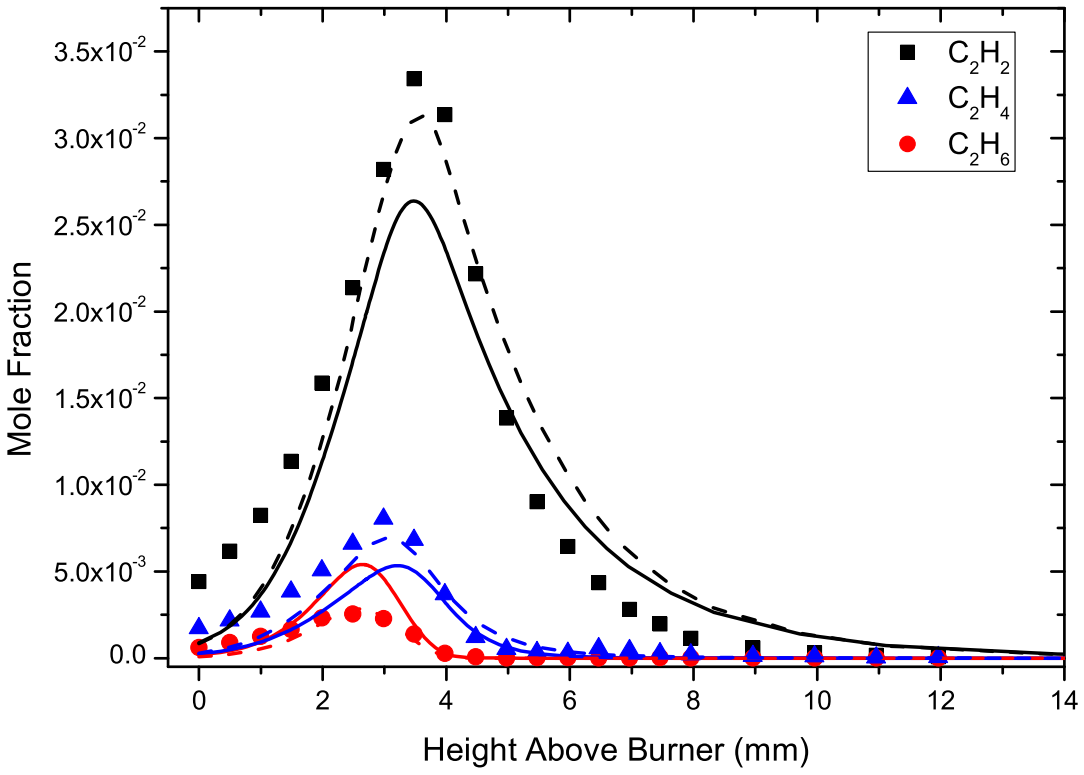

Figure 53: Experimental profiles [8] for acetylene, ethylene and ethane measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

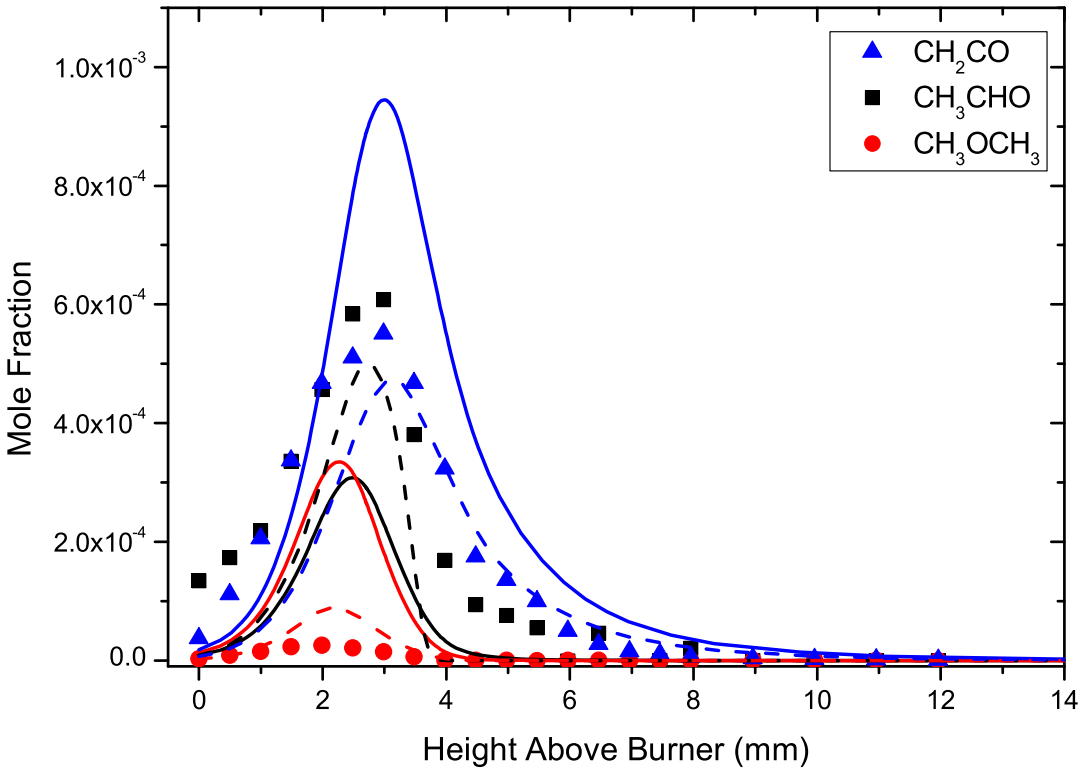

Figure 54: Experimental profiles [8] for ketene, acetaldehyde and dimethyl ether measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

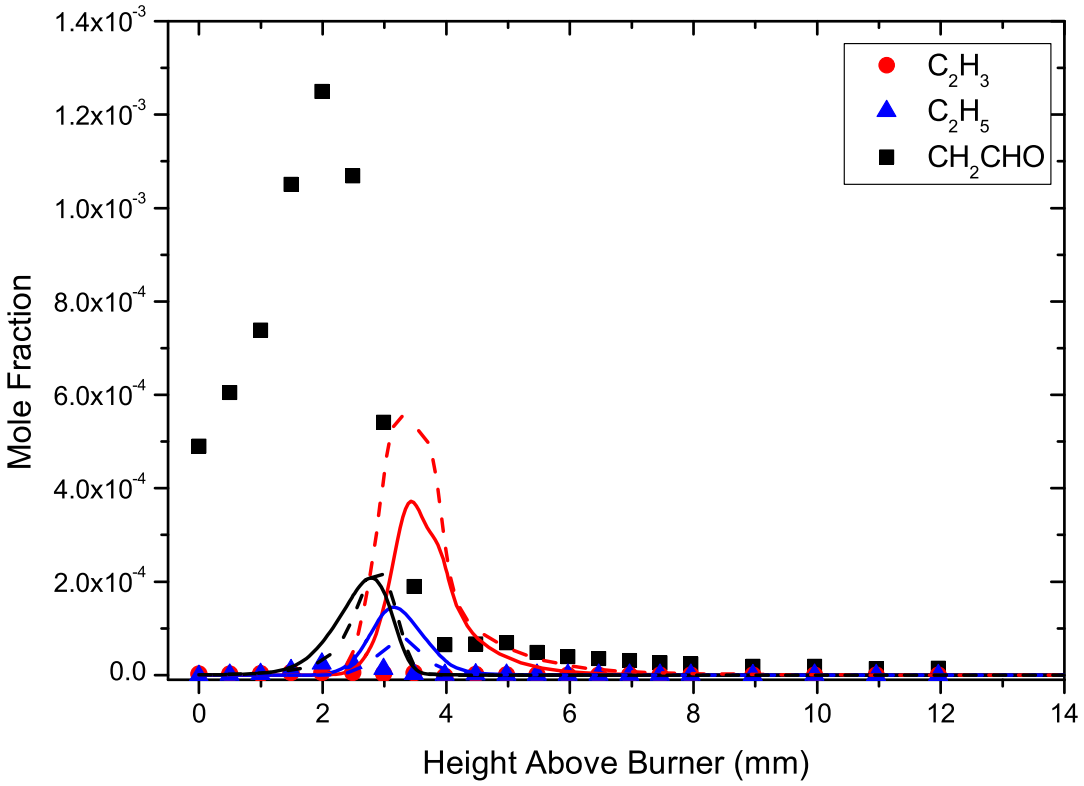

Figure 55: Experimental profiles [8] for vinyl, ethyl and vinoxy radicals measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

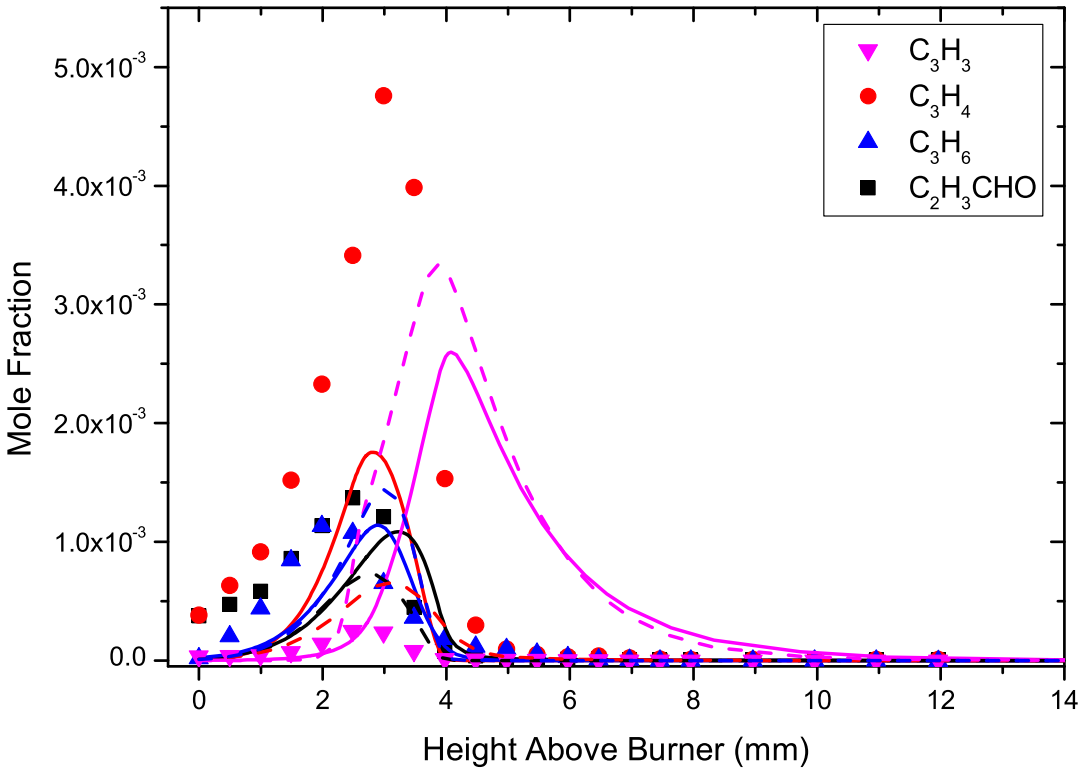

Figure 56: Experimental profiles [8] for propargyl radical, propyne, propene and acrolein measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

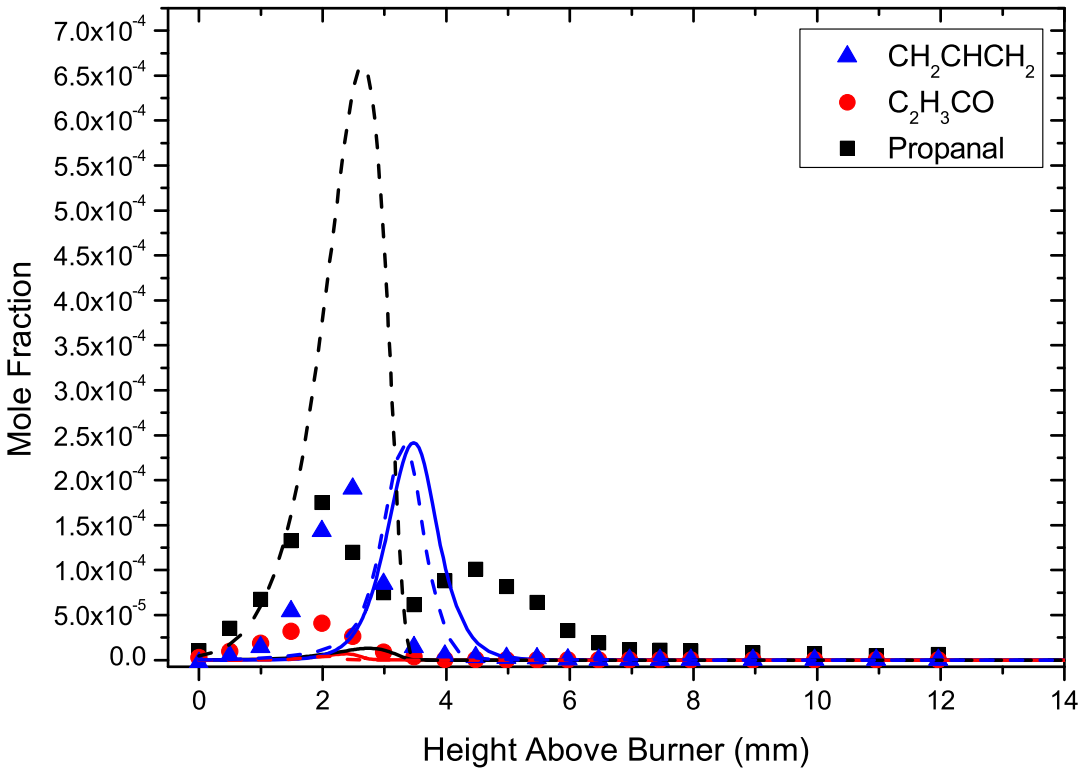

Figure 57: Experimental profiles [8] for allyl and acrolein radicals and propanal measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

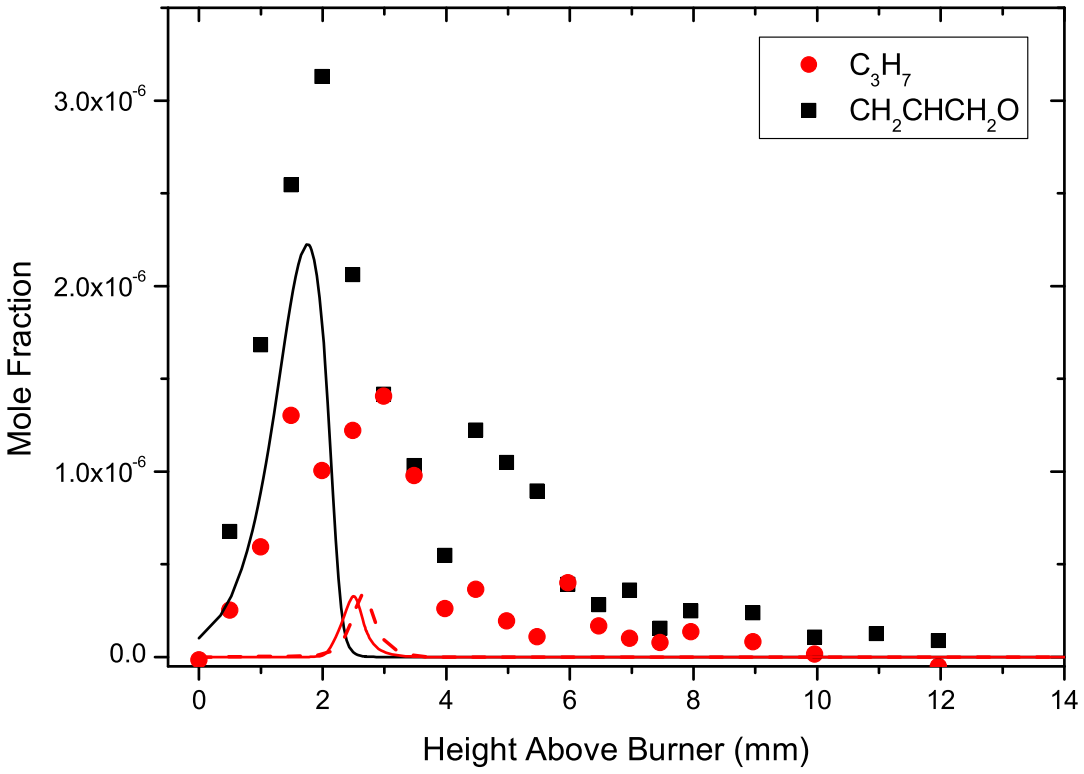

Figure 58: Experimental profiles [8] for *n*-propyl and allyloxy radicals measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

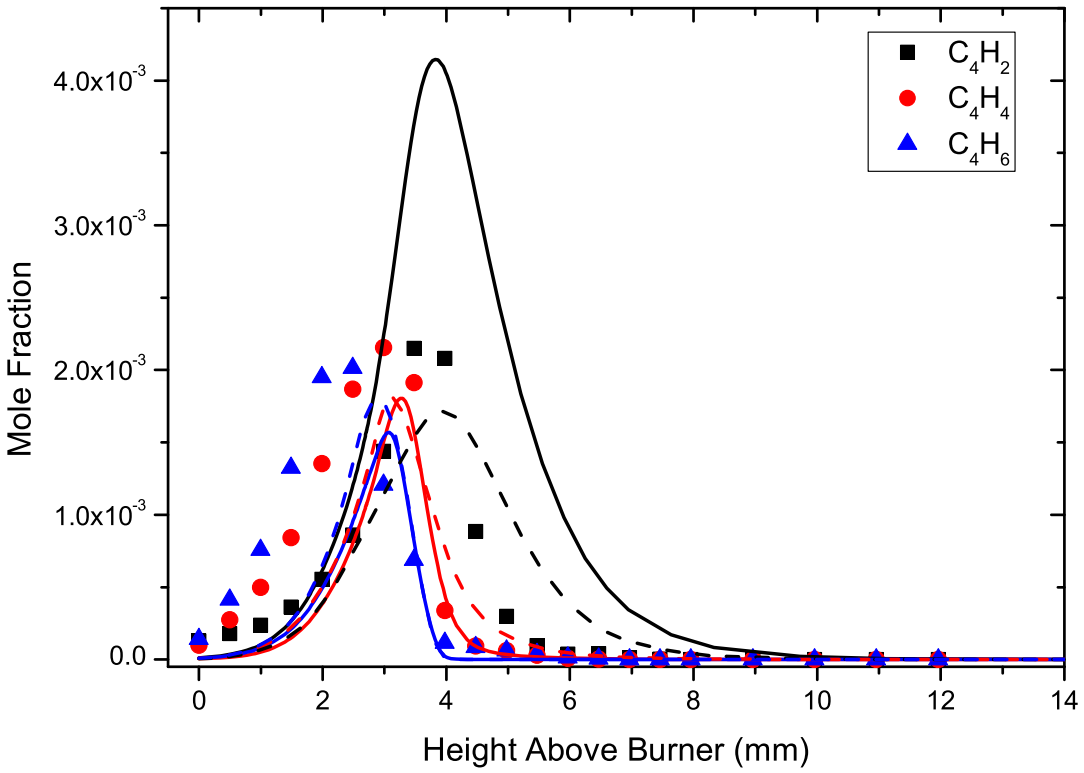

Figure 59: Experimental profiles [8] for diacetylene, vinylacetylene and 1,3-butadiene measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

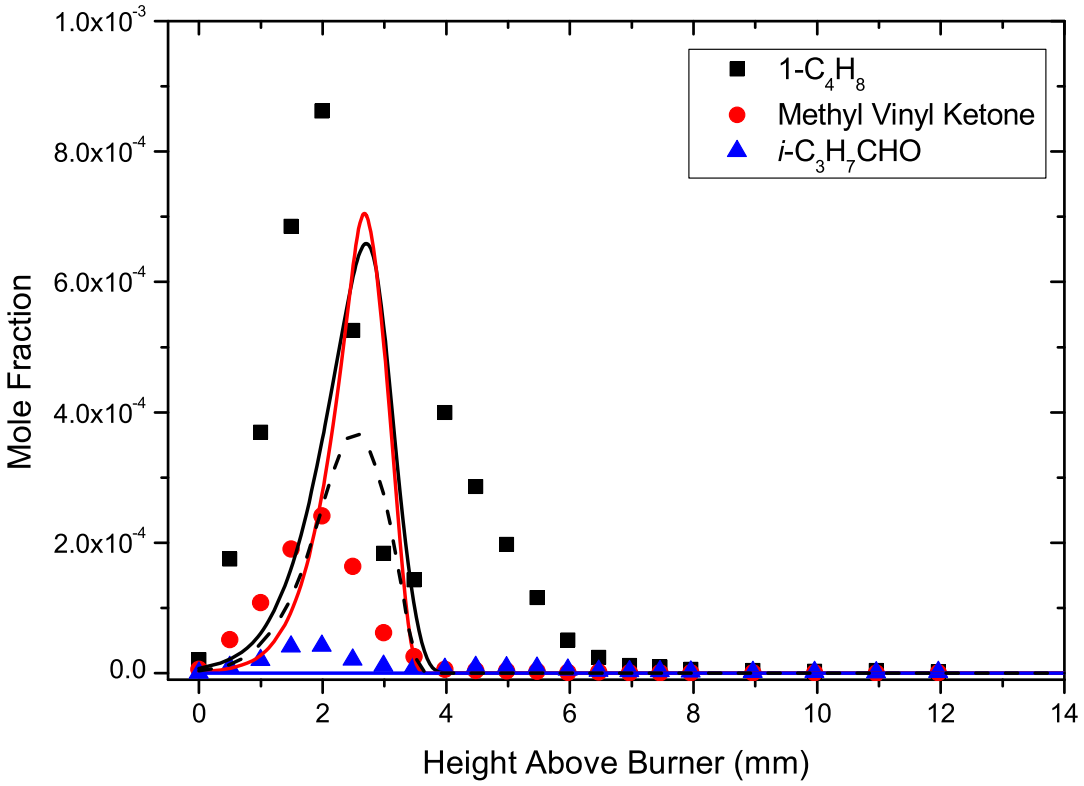

Figure 60: Experimental profiles [8] for 1-butene, methyl vinyl ketone and *i*-butanal measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

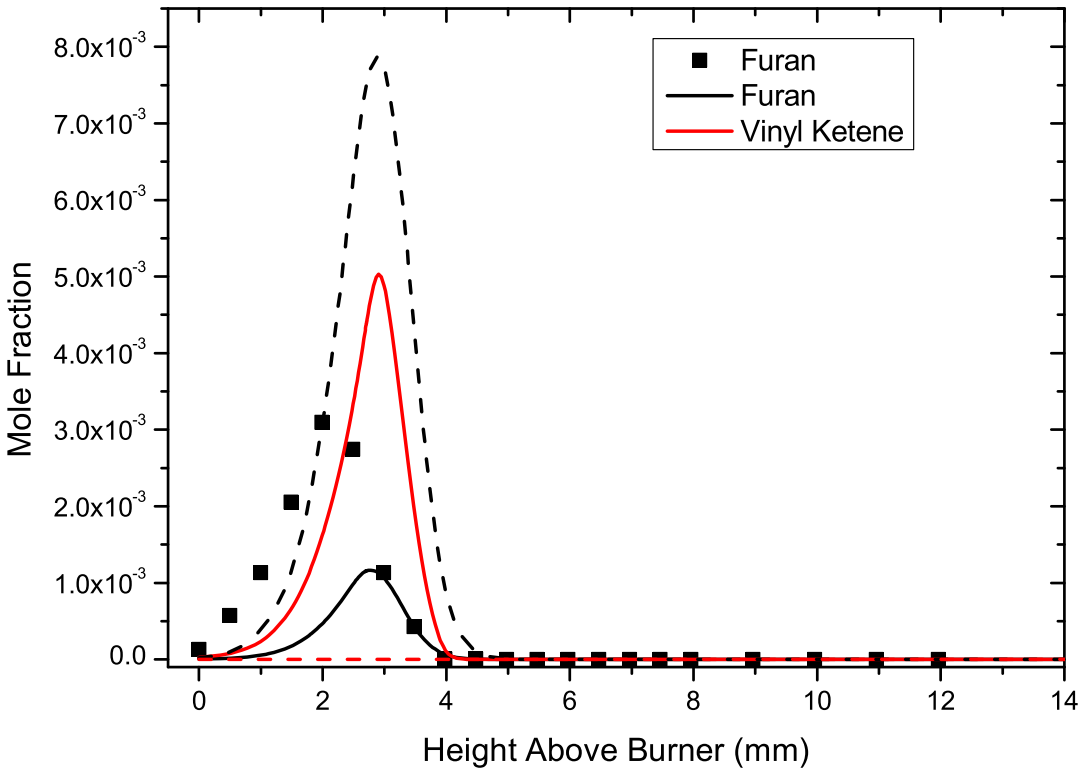

Figure 61: Experimental profile [8] for furan measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –). Vinyl ketene yields, which were not quantified experimentally, are included for comparison.

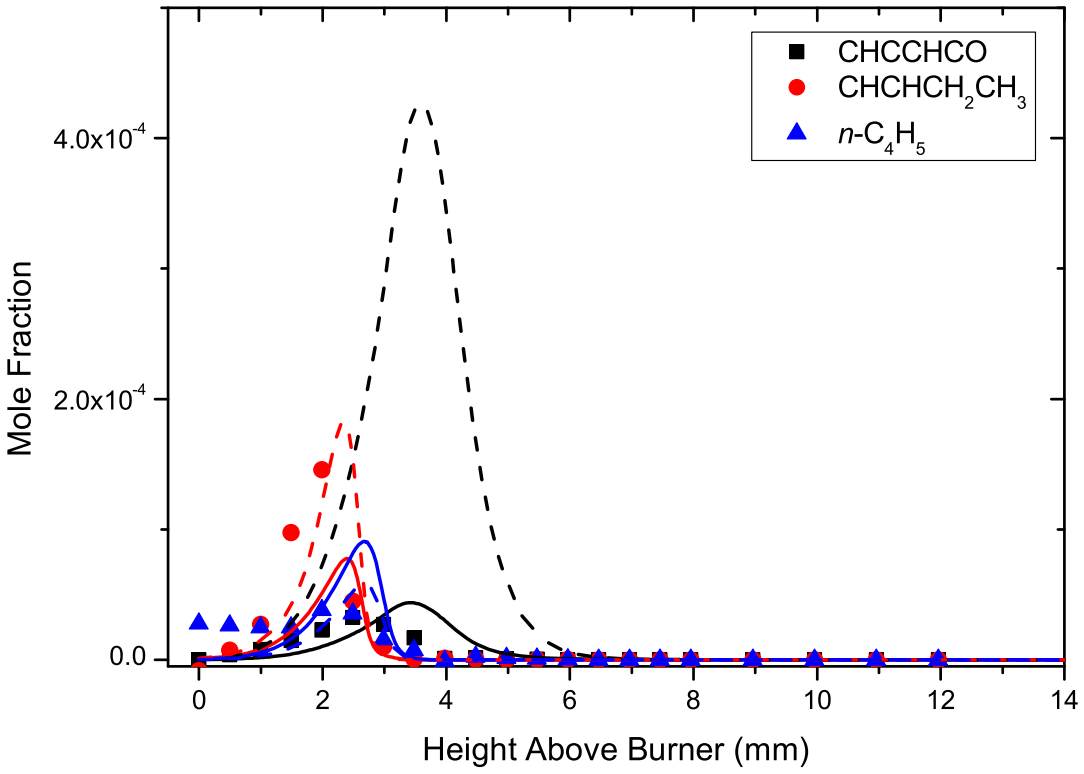

Figure 62: Experimental profiles [8] for acetylenylketene, *n*-butenyl and *n*-butadienyl measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

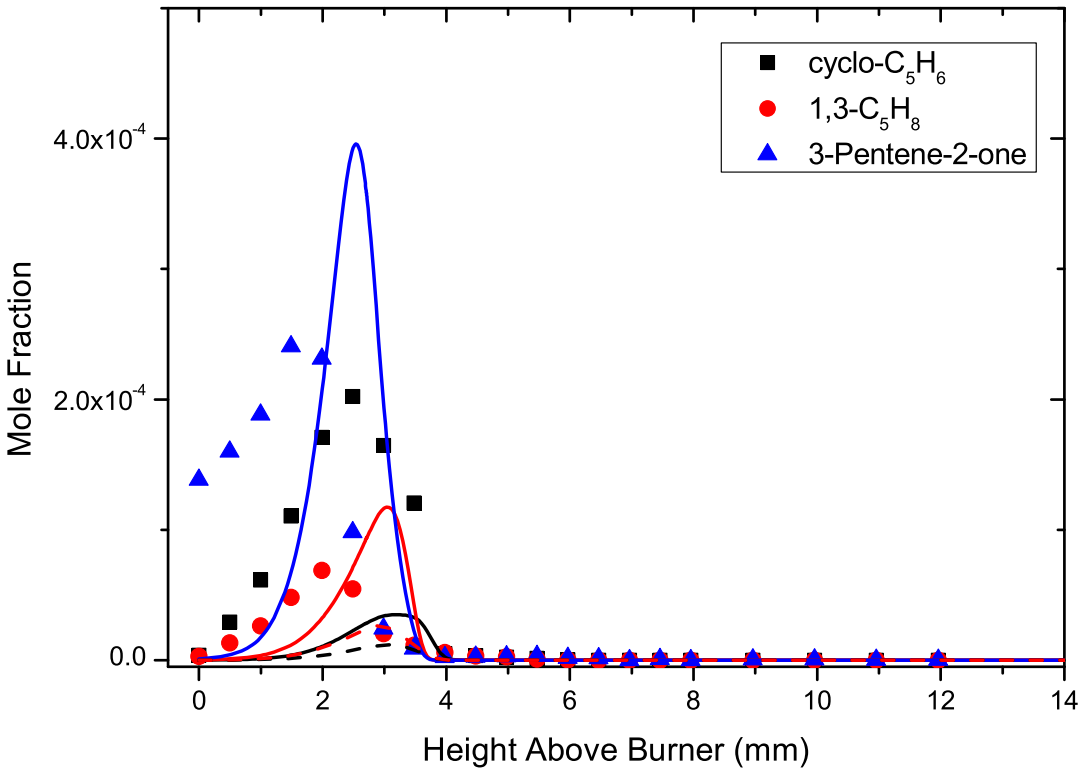

Figure 63: Experimental profiles [8] for 1,3-cyclopentadiene, 1,3-pentadiene and 3-pentene-2-one measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

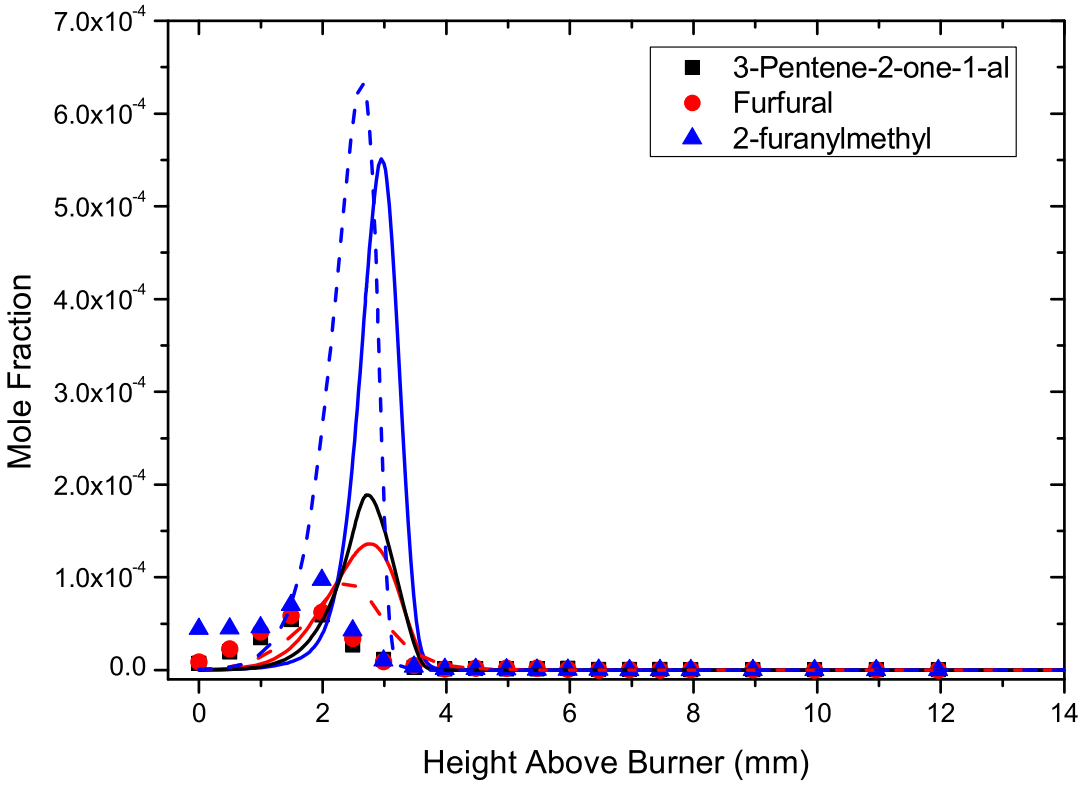

Figure 64: Experimental profiles [8] for 3-pentene-2-one-1-al, furfural and 2-furanylmethyl measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

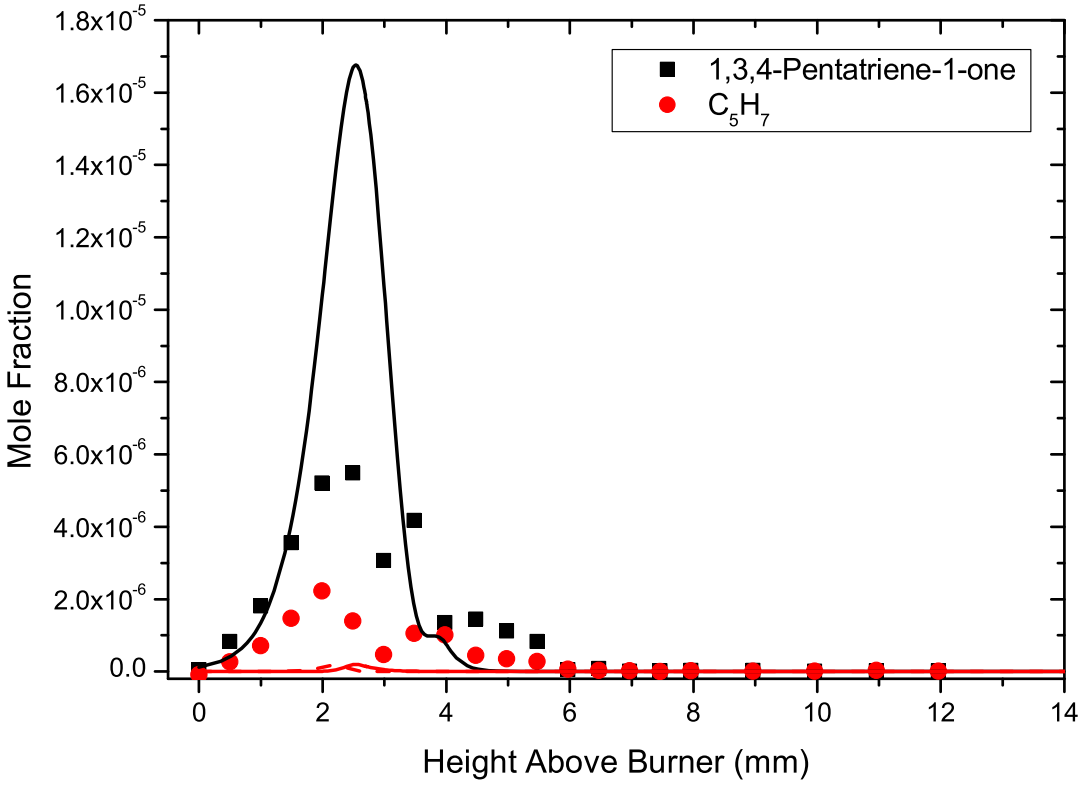

Figure 65: Experimental profiles [8] for 1,3,4-pentatriene-1-one and cyclopenteneyl radical measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

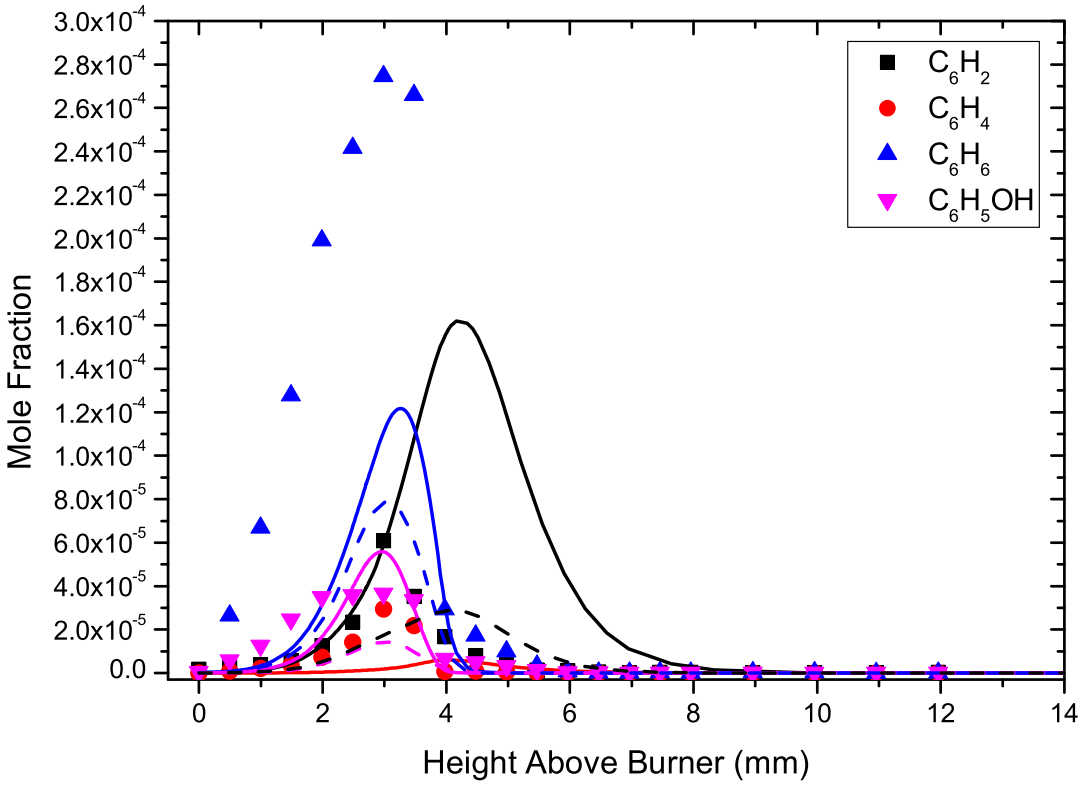

Figure 66: Experimental profiles [8] for triacetylene, benzyne, benzene and phenol measured in ϕ = 1.7 2-methylfuran/O_2/Ar flame with model calculations from *this work* (—) and the study of Tran *et al.* [8] (– –).

7 Electronic Energies of Stationary Points

Table 7: Electronic energies of potential energy surface minima (hartrees) at 0 and 298.15 K, at the CBS-QB3, G3 and CBS-APNO levels of theory.

	0 K			298 K		
SPECIES KEY	CBS-QB3	CBS-APNO	G3	CBS-QB3	CBS-APNO	G3
M1	-268.878010	-269.239467	-269.140183	-268.871675	-269.233241	-269.133826
M2	-268.780525	-269.141719	-269.043882	-268.774038	-269.135313	-269.037350
M3	-268.790419	-269.151663	-269.053756	-268.783748	-269.145113	-269.047076
M4		-269.140879	-269.043143		-269.134552	-269.036692
M5	-268.828555	-269.189009	-269.092552	-268.820712	-269.181216	-269.084637
M6	-268.833058	-269.193615	-269.097062	-268.825259	-269.185891	-269.089199
M7	-268.787268	-269.148816	-269.050872	-268.780430	-269.142226	-269.044166
M8	-268.837026	-269.197901	-269.101105	-268.829150	-269.190105	-269.093191
M9	-268.840399	-269.201196	-269.104571	-268.832544	-269.193440	-269.096683
M10	-268.242558	-268.603230	-268.502648	-268.236633	-268.597206	-268.496472
M11	-268.196518	-268.556205	-268.457185	-268.189076	-268.548544	-268.449384
M12	-268.198158	-268.557780	-268.458999	-268.190710	-268.550103	-268.451174
M13	-268.219529	-268.580434	-268.482047	-268.212108	-268.572919	-268.474365
M14	-268.208236			-268.200944		
M15	-268.218942	-268.580115	-268.481620	-268.211640	-268.572689	-268.474032
M16	-268.252517	-268.613698	-268.513834	-268.246553	-268.607680	-268.507688
INT1	-267.571448	-267.932155	-267.834361	-267.565545	-267.926013	-267.828070
M17	-269.426024	-269.788171	-269.689663	-269.419313	-269.781369	-269.682704
M18	-269.419453	-269.780791	-269.683088	-269.411631	-269.772651	-269.674835
M19	-269.422043	-269.783263	-269.685168	-269.414092	-269.775271	-269.677043
M20	-269.413783	-269.776428		-269.405853	-269.768529	
M21	-269.427416	-269.788712	-269.691038	-269.419638	-269.780759	-269.682943
M22	-269.426484	-269.787669	-269.689808	-269.418482	-269.779554	-269.681562
M23	-269.428124	-269.790975	-269.691527	-269.420239	-269.782884	-269.683333
M24	-269.415684	-269.777058	-269.680532	-269.407798	-269.769087	-269.672401
M25	-269.415089	-269.776869	-269.680052	-269.407249	-269.768921	-269.671971
M26	-269.413862	-269.775588	-269.676084	-269.406485	-269.767901	-269.668250
M27	-269.425835	-269.787791	-269.689875	-269.419137	-269.780990	-269.682923
M28	-269.408650	-269.770785	-269.671905	-269.401728	-269.763978	-269.664959
M29	-269.381422	-269.742612	-269.646344	-269.372996	-269.734233	-269.637806
M30	-269.383034	-269.744449	-269.648290	-269.374692	-269.736172	-269.639862
M31	-269.382326	-269.743711	-269.647581	-269.373964	-269.735414	-269.639119
M32	-269.407525	-269.769347	-269.671789	-269.399593	-269.761489	-269.663765
M33	-269.407433	-269.769275		-269.399482	-269.761382	
M34	-269.428082	-269.790832	-269.692642	-269.421092	-269.783930	-269.685582
M35	-269.407639	-269.770444	-269.672986	-269.399634	-269.762501	-269.664909
M36	-269.410042	-269.772122	-269.673673	-269.403112	-269.765325	-269.666743
M37	-269.379642	-269.740604	-269.644070	-269.371172	-269.732068	-269.635386
M38	-269.380945	-269.742131	-269.645575	-269.372547	-269.733722	-269.637029
M39	-269.382060	-269.743034	-269.646592	-269.373606	-269.734593	-269.638004
M40	-269.412609	-269.775079	-269.677128	-269.404353	-269.766854	-269.668761
M41	-269.428563	-269.790408	-269.691568	-269.421611	-269.783345	-269.684359
M42	-269.431395	-269.792770	-269.695758	-269.423471	-269.784789	-269.687634
M43	-269.428054	-269.789416	-269.692063	-269.420328	-269.781622	-269.684128
M44	-269.410349	-269.771902	-269.672273	-269.402454	-269.763992	-269.664221
M45	-269.412705	-269.774042	-269.674618	-269.404677	-269.765995	-269.666431
M46	-269.371297	-269.733934	-269.635435	-269.363147	-269.725758	-269.627143
M47	-269.409124	-269.772176		-269.400918	-269.763967	
M48	-269.410381	-269.772863		-269.402134	-269.764632	

Table 8: Electronic energies of transition states (hartrees) at 0 and 298.15 K, at the CBS-QB3, G3 and CBS-APNO levels of theory.

	0 K			298 K		
SPECIES KEY	CBS-QB3	CBS-APNO	G3	CBS-QB3	CBS-APNO	G3
TS1	-268.746128	-269.107874	-269.008275	-268.740121	-269.101944	-269.002235
TS2	-268.773442	-269.136209	-269.036282	-268.767167	-269.130023	-269.029972
TS3	-268.736922	-269.097899	-268.999123	-268.729195	-269.090488	-268.991566
TS4	-268.742039	-269.103398	-269.004371	-268.734061	-269.095741	-268.996592
TS5	-268.765437	-269.127648	-269.028449	-268.759340	-269.121616	-269.022294
TS6		-269.141949	-269.044112		-269.135611	-269.037656
TS7	-268.820518	-269.180773	-269.084361	-268.813204	-269.173574	-269.077045
TS8	-268.763132	-269.124961		-268.755571	-269.117871	
TS9	-268.733495		-268.999152	-268.725922		-268.990439
TS10	-268.767849	-269.130172	-269.030746	-268.761602	-269.124020	-269.024476
TS11	-268.785869	-269.148513	-269.050644	-268.779309	-269.142682	-269.043801
TS12	-268.830516	-269.190787	-269.094588	-268.823329	-269.183716	-269.087389
TS13	-268.730957	-269.095001	-268.995346	-268.723270	-269.087148	-268.987478
TS14	-268.178692			-268.172433		
TS15	-268.112920	-268.473401		-268.104830	-268.465089	
TS16	-268.182698	-268.542470	-268.445277	-268.175565	-268.535099	-268.437750
TS17	-268.159951	-268.521173	-268.420075	-268.153223	-268.514191	-268.412942
TS18	-268.206930			-268.199944		
TS19	-268.170360			-268.161919		
TS20	-268.202003	-268.563008	-268.466357	-268.194987	-268.555959	-268.459123
TS21	-268.200554	-268.559642		-268.194340	-268.553295	
TS22	-268.164829	-268.522351	-268.424624	-268.157818	-268.515558	-268.417652
TS23a	-267.546464	-267.907822	-267.807266	-267.540672	-267.902207	-267.801553
TS23b	-267.562621	-267.925368	-267.826986	-267.556788	-267.919413	-267.820903
TS24	-269.373163	-269.734491	-269.637586	-269.366305	-269.727653	-269.630582
TS25	-269.376918	-269.742674	-269.639333	-269.369585	-269.735143	-269.631822
TS26	-269.387892		-269.653768	-269.381358		-269.647004
TS27	-269.410890			-269.403242		
TS28	-269.374059	-269.738351		-269.366838	-269.730931	
TS29	-269.374986			-269.365906		
TS30	-269.391722		-269.656570	-269.384961		-269.649555
TS31	-269.413417	-269.774823	-269.678314	-269.405852	-269.767189	-269.670551
TS32	-269.375835	-269.738354		-269.368472	-269.730935	
TS33	-269.407053			-269.399739		
TS34	-269.363161		-269.626267	-269.355898		-269.618977
TS35	-269.412277	-269.773763	-269.676817	-269.405105	-269.766518	-269.669444
TS36	-269.364913			-269.356503		
TS37	-269.387089			-269.380657		
TS38	-269.354847	-269.716069		-269.347955	-269.708892	
TS39	-269.367642	-269.732494	-269.634278	-269.360573	-269.725327	-269.626942
TS40	-269.371151	-269.732199	-269.634047	-269.364094	-269.725194	-269.626882
TS41	-269.354972	-269.717347	-269.617813	-269.347845	-269.710280	-269.610590
TS42	-269.380722	-269.741929	-269.645722	-269.373264	-269.734504	-269.638155
TS43	-269.377260	-269.739114	-269.643047	-269.369064	-269.730871	-269.634623
TS44	-269.343865	-269.705182	-269.607780	-269.334910	-269.696102	-269.598493
TS45	-269.367034	-269.730287	-269.631275	-269.360109	-269.723315	-269.624150
TS46	-269.404123	-269.765792		-269.396928	-269.758647	
TS47	-269.353030	-269.717239		-269.343925	-269.707691	
TS48	-269.378690	-269.741084	-269.642710	-269.371989	-269.734258	-269.635746
TS49	-269.373026	-269.73388	-269.63722	-269.36597	-269.727	-269.6302

Table 8: Electronic energies of transition states (hartrees) at 0 and 298.15 K, at the CBS-QB3, G3 and CBS-APNO levels of theory.

	0 K			298 K		
SPECIES KEY	CBS-QB3	CBS-APNO	G3	CBS-QB3	CBS-APNO	G3
TS50	-269.37811	-269.73877	-269.64237	-269.37108	-269.73188	-269.63536
TS51	-269.385097	-269.74764	-269.64883	-269.37827	-269.74076	-269.64181
TS52	-269.384934	-269.747059	-269.649809	-269.376235	-269.738711	-269.641320
TS53	-269.370262	-269.73152	-269.63352	-269.36327	-269.72456	-269.6264
TS54	-269.354953	-269.71717	-269.61723	-269.34776	-269.70998	-269.60989
TS55	-269.379522	-269.74044	-269.64393	-269.37186	-269.73275	-269.6361
TS56	-269.345266	-269.70628	-269.60805	-269.33647	-269.69728	-269.59888
TS57	-269.378011	-269.7389	-269.64236	-269.37019	-269.73111	-269.63445
TS58	-269.365541	-269.72791	-269.62847	-269.35782	-269.72024	-269.62065
TS59	-269.400480	-269.762863	-269.664487	-269.392072	-269.754421	-269.655913
TS60	-269.37516	-269.73576	-269.63883	-269.36789	-269.72868	-269.63158
TS61	-269.393982			-269.38721		
TS62	-269.35303	-269.71724		-269.34393	-269.70769	
TS63	-269.421257	-269.78309	-269.68674	-269.41391	-269.77571	-269.67921
TS64	-269.380615			-269.3735		
TS65	-269.407735			-269.40046		
TS66	-269.338546	-269.70256	-269.60613	-269.32958	-269.694	-269.59737
TS67	-269.369328	-269.73206	-269.63502	-269.36156	-269.72418	-269.62701
TS68	-269.366156	-269.72932	-269.63061	-269.3586	-269.72164	-269.62278
TS69	-269.408708			-269.4012		
TS70	-269.399381	-269.76199	-269.66354	-269.39098	-269.75359	-269.65499

Table 9: Electronic energies of fragmentation products (hartrees) at 0 and 298.15 K, at the CBS-QB3, G3 and CBS-APNO levels of theory.

	0 K			298 K		
SPECIES KEY	CBS-QB3	CBS-APNO	G3	CBS-QB3	CBS-APNO	G3
P1	-191.599268	-191.845578	-191.775326	-191.593607	-191.839978	-191.769643
P2	-77.187419	-77.301546	-77.275962	-77.183653	-77.297904	-77.272274
P3	-152.375854	-152.563747	-152.506868	-152.371390	-152.559357	-152.502428
P4	-116.421682	-116.595023	-116.555356	-116.416763	-116.590234	-116.550501
P5	-155.646207	-155.877658	-155.825190	-155.640225	-155.871804	-155.819230
P6	-113.182008	-113.311629	-113.267369	-113.178703	-113.308324	-113.264064
P7	-155.648350	-155.879729	-155.827386	-155.642329	-155.873765	-155.821333
P8	-155.008157	-155.239852	-155.185648	-155.001788	-155.233378	-155.179038
P9	-113.704761	-113.835367	-113.791540	-113.700959	-113.831568	-113.787739
P10	-39.744800	-39.803679	-39.793293	-39.740785	-39.799517	-39.789047
P11	-228.963076	-229.265558	-229.179231	-228.956860	-229.259312	-229.172852
P12	-228.965879	-229.268213	-229.182184	-228.959574	-229.261867	-229.175706
P13	-152.942049	-153.131169	-153.073738	-152.937133	-153.126240	-153.068768
P14	-115.778670	-115.951756	-115.911633	-115.773628	-115.946653	-115.906398
P15	-228.958465	-229.260954		-228.951912	-229.254681	
P16	-228.960097	-229.262597		-228.953791	-229.256365	
P17	-0.499818	-0.499946	-0.501003	-0.497457	-0.497585	-0.498642
P18	-267.618427	-267.978869	-267.880816	-267.611059	-267.971636	-267.873455
P19	-154.991766	-155.223308	-155.168855	-154.986126	-155.217479	-155.163060
P20	-267.663797	-268.024160	-267.925018	-267.658107	-268.018546	-267.919292
P21	-151.708757	-151.897602	-151.840730	-151.704285	-151.892633	-151.835687

Table 9: Electronic energies of fragmentation products (hartrees) at 0 and 298.15 K, at the CBS-QB3, G3 and CBS-APNO levels of theory.

	0 K			298 K		
SPECIES KEY	CBS-QB3	CBS-APNO	G3	CBS-QB3	CBS-APNO	G3
P22	-229.643105	-229.946256	-229.859940	-229.638424	-229.941643	-229.855244
P23	-156.196597	-156.428403	-156.377094	-156.190323	-156.422134	-156.370723
P24	-155.662340	-155.893410	-155.841379	-155.656670	-155.887776	-155.835664
P25	-75.649720	-75.723054	-75.694904	-75.646415	-75.719750	-75.691600
P26	-193.712772	-194.002045	-193.933769	-193.707641	-193.996961	-193.928586
P27	-192.168433	-192.414918	-192.344792	-192.162382	-192.408912	-192.338706
P28	-117.009514	-117.183147	-117.144897	-117.004726	-117.178269	-117.139937
P29	-268.876456	-269.238313	-269.139753	-268.870251	-269.232171	-269.133501
P30	-268.882498	-269.244390	-269.145813	-268.876332	-269.238235	-269.139558
P31	-156.211316	-156.443511		-156.204705	-156.436817	
P32	-152.932833	-153.120583	-153.063707	-152.928348	-153.116108	-153.059187
P33	-156.239817	-156.471904	-156.419916	-156.233541	-156.465498	-156.413404
P34	-229.618062	-229.921239	-229.837341	-229.611692	-229.914963	-229.830972
P35	-116.971430	-117.144744	-117.106687	-116.966319	-117.139622	-117.101499
P36	-156.238812	-156.471114	-156.418959	-156.232480	-156.464603	-156.412360

8 Geometries of Stationary Points

Table 10: Cartesian coordinates for minima (M1–M9) on the C_5H_6O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M1 CBS-QB3				M1 CBS-APNO				M1 G3		
6	-1.3972860	-0.7320440	-0.0003310	6	1.3927340	-0.7385560	0.0000170	6	1.3850100	-0.7244670	0.0002030
6	-1.5470180	0.6156580	0.0000750	6	1.5467530	0.6161820	-0.0000140	6	1.5442920	0.6037180	-0.0000830
6	-0.2201260	1.1624850	-0.0002060	6	0.2301130	1.1648740	0.0000110	6	0.2133730	1.1545860	0.0003150
6	0.6385010	0.1064790	-0.0000320	6	-0.6394200	0.1094460	-0.0000160	6	-0.6260720	0.1065660	0.0000970
8	-0.0724600	-1.0625710	0.0004010	1	2.0790690	-1.5719760	0.0000040	1	2.0691420	-1.5445490	0.0002030
1	-2.0866490	-1.5590600	-0.0005010	1	2.4846490	1.1541030	0.0000200	1	2.4719150	1.1378390	-0.0002960
1	-2.4790830	1.1581260	0.0001350	1	-0.0435490	2.2113760	-0.0000100	1	-0.0610060	2.1896860	0.0004070
1	0.0551460	2.2054040	-0.0003490	8	0.0660410	-1.0659870	-0.0000080	8	0.0770890	-1.0428640	0.0003130
6	2.1200270	-0.0142950	0.0000460	6	-2.1193260	-0.0110440	0.0000050	6	-2.1165790	-0.0193690	0.0001650
1	2.4752220	-0.5550800	0.8829750	1	-2.4740500	-0.5483110	0.8845330	1	-2.5025150	-0.1257360	1.0083890
1	2.4752730	-0.5555600	-0.8825670	1	-2.5655000	0.9857600	-0.0000740	1	-2.5851070	0.8513660	-0.4460060
1	2.5751800	0.9770390	-0.0002120	1	-2.4740680	-0.5484650	-0.8844210	1	-2.4092830	-0.8919000	-0.5693880
	M2 CBS-QB3				M2 CBS-APNO				M2 G3		
6	-0.1492760	-1.2416440	0.1830600	6	-0.1574110	-1.2280120	0.1900220	6	-0.1551530	-1.2325270	0.1951300
6	0.6815710	0.0063920	0.4390310	6	0.6836120	0.0079400	0.4547540	6	0.6835270	0.0092230	0.4594380
6	-0.2536920	1.1552460	0.1549810	6	-0.2577760	1.1469470	0.1576080	6	-0.2573180	1.1481060	0.1606530
6	-1.4188330	0.6287560	-0.1820400	6	-1.3989870	0.6079270	-0.1860600	6	-1.3982930	0.6087610	-0.1881440
8	-1.3452150	-0.8022600	-0.1550200	8	-1.3322350	-0.7853810	-0.1583960	8	-1.3317560	-0.7849960	-0.1603980
1	0.9110130	-0.0409230	1.5166180	1	0.9236360	-0.0320510	1.5188300	1	0.9331640	-0.0250440	1.5209740
1	-0.0227870	2.2077000	0.2191990	1	-0.0445030	2.1948110	0.2175250	1	-0.0399470	2.1950730	0.2216700
6	2.0118060	-0.0057190	-0.3358600	6	1.9925310	-0.0095000	-0.3440820	6	1.9883090	-0.0096400	-0.3486250
1	2.5737770	-0.9099290	-0.0978140	1	2.5696150	-0.8930010	-0.0984830	1	2.5664580	-0.8934350	-0.1081970
1	1.8314750	0.0108900	-1.4128800	1	1.7953280	-0.0163360	-1.4112330	1	1.7851730	-0.0146730	-1.4140530
1	2.6187630	0.8644300	-0.0763860	1	2.5883520	0.8683030	-0.1167430	1	2.5876000	0.8660980	-0.1250460
1	-2.3799750	1.0277260	-0.4636120	1	-2.3463620	1.0095070	-0.4761880	1	-2.3448350	1.0084140	-0.4828710
	M3 CBS-QB3				M3 CBS-APNO				M3 G3		
6	0.6439790	0.1579560	0.0024620	6	0.6439790	0.1579560	0.0024620	6	0.6439790	0.1579560	0.0024620
6	-0.2642690	1.1345250	0.0043940	6	-0.2642690	1.1345250	0.0043940	6	-0.2642690	1.1345250	0.0043940
6	-1.3527320	-1.0005910	-0.0097340	6	-1.3527320	-1.0005910	-0.0097340	6	-1.3527320	-1.0005910	-0.0097340
8	-0.0358480	-1.1155640	-0.0012160	8	-0.0358480	-1.1155640	-0.0012160	8	-0.0358480	-1.1155640	-0.0012160
1	-0.0520920	2.1960150	0.0043090	1	-0.0520920	2.1960150	0.0043090	1	-0.0520920	2.1960150	0.0043090
6	2.1212890	0.0588870	-0.0002950	6	2.1212890	0.0588870	-0.0002950	6	2.1212890	0.0588870	-0.0002950
1	2.4726270	-0.4797900	0.8843310	1	2.4726270	-0.4797900	0.8843310	1	2.4726270	-0.4797900	0.8843310

Table 10: Cartesian coordinates for minima (M1–M9) on the C_5H_6O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.4678030	-0.4870240	-0.8824530	1	2.4678030	-0.4870240	-0.8824530	1	2.4678030	-0.4870240	-0.8824530
1	2.5650550	1.0562690	-0.0054050	1	2.5650550	1.0562690	-0.0054050	1	2.5650550	1.0562690	-0.0054050
6	-1.6168070	0.4953470	-0.0077500	6	-1.6168070	0.4953470	-0.0077500	6	-1.6168070	0.4953470	-0.0077500
1	-2.1697440	0.6988660	0.9232880	1	-2.1697440	0.6988660	0.9232880	1	-2.1697440	0.6988660	0.9232880
1	-2.1856170	0.8634390	-0.8487990	1	-2.1856170	0.8634390	-0.8487990	1	-2.1856170	0.8634390	-0.8487990
	M4 CBS-APNO				M4 G3						
6	0.6573740	0.1104670	0.4573750	6	0.6568900	0.1088130	0.4618080				
6	-0.2090140	1.2888490	0.1939490	6	-0.2068130	1.2916710	0.2001730				
6	-1.4316920	0.6976830	-0.1856940	6	-1.4283190	0.6985240	-0.1877020				
6	-1.2988450	-0.6637620	-0.1646530	6	-1.3000660	-0.6619700	-0.1675370				
8	-0.1373900	-1.0963620	0.1862150	8	-0.1365920	-1.0994860	0.1895520				
1	0.8785540	0.0704110	1.5188170	1	0.8861040	0.0613780	1.5202840				
1	-2.3345090	1.2064250	-0.4609980	1	-2.3298130	1.2084060	-0.4664030				
6	1.9273750	0.0388620	-0.3716220	6	1.9227290	0.0395900	-0.3763490				
1	2.5597510	0.8833120	-0.1289190	1	2.5538970	0.8871790	-0.1434640				
1	2.4620900	-0.8811160	-0.1657860	1	2.4646310	-0.8756760	-0.1713280				
1	1.6922830	0.0772350	-1.4298020	1	1.6798420	0.0709870	-1.4323290				
1	-2.0302340	-1.4179680	-0.3991580	1	-2.0284550	-1.4161480	-0.4055390				
	M5 CBS-QB3				M5 CBS-APNO				M5 G3		
6	1.5424880	0.1460880	0.5420400	6	1.5288190	0.1496570	0.5433010	6	1.5295850	0.1485540	0.5446340
6	0.3640730	0.5686210	0.1949000	6	0.3580180	0.5616530	0.1930950	6	0.3561110	0.5605850	0.1953100
6	-0.8385120	0.9690990	-0.1515840	6	-0.8314760	0.9650180	-0.1561800	6	-0.8342880	0.9661800	-0.1552400
6	-2.0172880	0.0644720	-0.1621670	6	-2.0059590	0.0550690	-0.1608510	6	-2.0068160	0.0579010	-0.1624360
8	-2.0079780	-1.1067240	0.1314010	8	-1.9863410	-1.0909530	0.1332740	8	-1.9851350	-1.0942690	0.1331310
1	1.8108530	0.2111130	1.5958380	1	1.7878120	0.2256820	1.5879310	1	1.7933080	0.2213870	1.5876870
1	-1.0118410	2.0024640	-0.4446110	1	-0.9927700	1.9878020	-0.4534910	1	-0.9949380	1.9892090	-0.4513340
6	2.5680510	-0.4395150	-0.3968000	6	2.5502830	-0.4395180	-0.3954420	6	2.5516140	-0.4373840	-0.3965590
1	3.4926860	0.1450350	-0.3679680	1	3.4644680	0.1459290	-0.3724150	1	3.4648600	0.1489150	-0.3767970
1	2.8162730	-1.4614550	-0.0951590	1	2.7954990	-1.4516570	-0.0894130	1	2.8020870	-1.4488140	-0.0939460
1	2.2015940	-0.4618490	-1.4231670	1	2.1796630	-0.4663530	-1.4119660	1	2.1802840	-0.4651100	-1.4126430
1	-2.9586210	0.5658890	-0.4744730	1	-2.9420500	0.5349420	-0.4703650	1	-2.9417570	0.5335440	-0.4722650
	M6 CBS-QB3				M6 CBS-APNO				M6 G3		
6	-1.7442360	-0.3319760	0.4333050	6	-1.7292250	-0.3340990	0.4339550	6	-1.7315030	-0.3356490	0.4339930
6	-0.5051300	-0.4734280	0.0622870	6	-0.4982040	-0.4651480	0.0648060	6	-0.4992680	-0.4696920	0.0629780

Table 10: Cartesian coordinates for minima (M1–M9) on the C_5H_6O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	0.7542570	-0.5860430	-0.2940800	6	0.7473990	-0.5855490	-0.2982960	6	0.7489110	-0.5866010	-0.2990220
6	1.7859190	0.3428240	0.2141530	6	1.7803340	0.3409380	0.2131850	6	1.7783140	0.3408650	0.2143100
8	2.9544920	0.2777440	-0.0871870	8	2.9241950	0.2767620	-0.0862680	8	2.9282830	0.2790080	-0.0855690
1	-2.0686320	-0.8651700	1.3262500	1	-2.0431810	-0.8714520	1.3156420	1	-2.0492420	-0.8695310	1.3156260
1	1.0910280	-1.3655710	-0.9727850	1	1.0654780	-1.3589050	-0.9764200	1	1.0714860	-1.3575800	-0.9769910
6	-2.7765530	0.5049200	-0.2811250	6	-2.7587270	0.5049170	-0.2792620	6	-2.7596110	0.5068870	-0.2785810
1	-3.6171130	-0.1181290	-0.6016320	1	-3.5892800	-0.1160860	-0.6010000	1	-3.5924140	-0.1091250	-0.6024680
1	-3.1764490	1.2718600	0.3890680	1	-3.1532570	1.2635400	0.3899020	1	-3.1539330	1.2665090	0.3888730
1	-2.3546080	0.9960410	-1.1581920	1	-2.3348390	0.9937850	-1.1470780	1	-2.3353800	0.9960490	-1.1457820
1	1.4042910	1.1212330	0.9075460	1	1.4120570	1.1086760	0.9027730	1	1.4121650	1.1067540	0.9032200
	M7 CBS-QB3				M7 CBS-APNO				M7 G3		
6	-1.5501020	0.8521630	0.0041880	6	-1.5501020	0.8521630	0.0041880	6	-1.5501020	0.8521630	0.0041880
6	-0.1994300	1.1927880	0.0053090	6	-0.1994300	1.1927880	0.0053090	6	-0.1994300	1.1927880	0.0053090
6	0.6184300	0.0510780	-0.0028530	6	0.6184300	0.0510780	-0.0028530	6	0.6184300	0.0510780	-0.0028530
8	-0.0439250	-1.0754660	-0.0081910	8	-0.0439250	-1.0754660	-0.0081910	8	-0.0439250	-1.0754660	-0.0081910
1	0.2158820	2.1962770	0.0050550	1	0.2158820	2.1962770	0.0050550	1	0.2158820	2.1962770	0.0050550
6	2.1024020	-0.0494040	-0.0024690	6	2.1024020	-0.0494040	-0.0024690	6	2.1024020	-0.0494040	-0.0024690
1	2.4372130	-0.5801770	0.8930390	1	2.4372130	-0.5801770	0.8930390	1	2.4372130	-0.5801770	0.8930390
1	2.4375530	-0.6224150	-0.8710450	1	2.4375530	-0.6224150	-0.8710450	1	2.4375530	-0.6224150	-0.8710450
1	2.5558060	0.9422340	-0.0245310	1	2.5558060	0.9422340	-0.0245310	1	2.5558060	0.9422340	-0.0245310
6	-1.5206660	-0.6101310	-0.0064930	6	-1.5206660	-0.6101310	-0.0064930	6	-1.5206660	-0.6101310	-0.0064930
1	-1.8952870	-1.0259690	0.9362640	1	-1.8952870	-1.0259690	0.9362640	1	-1.8952870	-1.0259690	0.9362640
1	-2.1035740	-0.9251890	-0.8593450	1	-2.1035740	-0.9251890	-0.8593450	1	-2.1035740	-0.9251890	-0.8593450
	M8 CBS-QB3				M8 CBS-APNO				M8 G3		
6	-2.2823030	-0.4727510	0.0000310	6	-2.2735410	-0.4639860	0.0002960	6	-2.2758370	-0.4642080	0.0003010
1	-2.3957270	-1.1127940	-0.8810010	1	-2.3832040	-1.0967410	-0.8764100	1	-2.3915150	-1.0967120	-0.8754130
1	-2.3959080	-1.1134660	0.8805430	1	-2.3825170	-1.0972860	0.8766870	1	-2.3915410	-1.0975010	0.8754290
1	-3.0557810	0.2933710	0.0002140	1	-3.0402760	0.2976740	0.0008090	1	-3.0411030	0.2989010	0.0006010
6	-0.9150690	0.1861580	0.0004050	6	-0.9100720	0.1874170	-0.0000920	6	-0.9099140	0.1845260	0.0006530
8	-0.7781950	1.3890190	-0.0001170	8	-0.7718660	1.3659350	-0.0001380	8	-0.7720500	1.3692040	-0.0003500
6	0.2477200	-0.7614490	-0.0002420	6	0.2505650	-0.7587480	-0.0003710	6	0.2493370	-0.7587870	-0.0008690
1	0.0366750	-1.8279650	-0.0003160	1	0.0529060	-1.8172370	-0.0008430	1	0.0506710	-1.8170020	-0.0007150
6	1.4912890	-0.3480210	-0.0001140	6	1.4814930	-0.3380100	-0.0000810	6	1.4823240	-0.3370330	-0.0002590
6	2.7160660	0.0803830	0.0000980	6	2.7002120	0.0820840	0.0002550	6	2.7039620	0.0803730	0.0004090

Table 10: Cartesian coordinates for minima (M1–M9) on the C_5H_6O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	3.2450660	0.2707790	0.9287330	1	3.2178990	0.2663780	0.9249960	1	3.2251140	0.2637060	0.9229730
1	3.2450160	0.2720010	-0.9283040	1	3.2181690	0.2671940	-0.9241740	1	3.2255410	0.2657570	-0.9214840
	M9 CBS-QB3				M9 CBS-APNO				M9 G3		
6	-0.9753250	1.4063990	0.0000250	6	-0.9883380	1.3966540	-0.0000180	6	-0.9812710	1.3982520	-0.0000220
1	-0.4334720	1.7639680	0.8798620	1	-0.4566130	1.7541040	0.8757140	1	-0.4495030	1.7573600	0.8746800
1	-0.4328720	1.7639010	-0.8794660	1	-0.4563370	1.7541250	-0.8755720	1	-0.4493170	1.7573670	-0.8746060
1	-1.9861330	1.8107460	-0.0003200	1	-1.9971640	1.7845220	-0.0001600	1	-1.9880040	1.7911620	-0.0001170
6	-1.0520410	-0.1072470	0.0000820	6	-1.0476490	-0.1129180	-0.0000130	6	-1.0459190	-0.1122960	-0.0000130
8	-2.1105370	-0.7000130	-0.0001290	8	-2.0794290	-0.7028190	0.0000490	8	-2.0862960	-0.6983710	0.0000610
6	0.2248670	-0.8837880	0.0002770	6	0.2323270	-0.8829280	-0.0000520	6	0.2291340	-0.8864350	-0.0000660
1	0.0979920	-1.9629920	-0.0006260	1	0.1260080	-1.9539640	-0.0000810	1	0.1186560	-1.9568100	-0.0001140
6	1.4230960	-0.3545520	0.0000130	6	1.4145910	-0.3426790	-0.0000190	6	1.4144950	-0.3477260	-0.0000170
6	2.6104840	0.1754220	-0.0000980	6	2.5932440	0.1856980	0.0000340	6	2.5934360	0.1841700	0.0000420
1	3.1263170	0.4032130	0.9277820	1	3.0972180	0.4103530	0.9237850	1	3.0996200	0.4109910	0.9216330
1	3.1259800	0.4038660	-0.9279930	1	3.0972680	0.4104470	-0.9236690	1	3.0996680	0.4111070	-0.9215000

Table 11: Cartesian coordinates for minima (M10–M16) on the C_5H_5O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M10 CBS-QB3				M10 CBS-APNO				M10 G3		
6	-1.3324220	-0.7272260	0.0005610	6	-1.3273830	-0.7233340	0.0004400	6	-1.3287010	-0.7246340	0.0004940
6	-1.4676890	0.6362810	-0.0003270	6	-1.4647080	0.6353550	-0.0000310	6	-1.4666490	0.6350560	-0.0000630
6	-0.1635750	1.1697930	-0.0000010	6	-0.1564570	1.1654880	-0.0001510	6	-0.1584730	1.1661000	-0.0001330
6	0.7295670	0.0804240	-0.0002570	6	0.7217530	0.0659990	-0.0000750	6	0.7227530	0.0679490	-0.0000860
8	-0.0215460	-1.0868460	-0.0003390	8	-0.0246150	-1.0759610	-0.0004230	8	-0.0235530	-1.0771200	-0.0004650
1	-2.0432010	-1.5365440	0.0008710	1	-2.0379940	-1.5206550	0.0005480	1	-2.0364390	-1.5242330	0.0006100
1	-2.3991490	1.1803090	-0.0000620	1	-2.3888520	1.1754670	0.0000370	1	-2.3904620	1.1761030	0.0000170
1	0.1232930	2.2092020	0.0005130	1	0.1367500	2.1948130	-0.0002890	1	0.1321550	2.1964380	-0.0002850
6	2.1008390	-0.0065140	-0.0000410	6	2.0958340	-0.0067430	0.0002200	6	2.0980010	-0.0059690	0.0002260
1	2.5930190	-0.9683850	0.0002300	1	2.5944370	-0.9565750	-0.0001670	1	2.5976950	-0.9547830	-0.0001200
1	2.6980770	0.8936340	0.0015420	1	2.6783410	0.8940540	0.0008360	1	2.6838850	0.8924310	0.0008700
	M11 CBS-QB3				M11 CBS-APNO				M11 G3		
6	1.0458270	0.9794320	0.0000230	6	1.0363760	0.9756390	0.0002600	6	1.0421120	0.9746780	0.0000120
6	-0.3502970	1.1878600	-0.0000420	6	-0.3644170	1.1868540	-0.0003380	6	-0.3590260	1.1869810	0.0000610
6	1.6998950	-0.3114300	0.0000280	6	1.7153310	-0.2996480	0.0002400	6	1.7186470	-0.2997160	0.0000900
6	-1.3119050	0.2545460	0.0000100	6	-1.3340720	0.2535700	-0.0002260	6	-1.3317590	0.2526390	-0.0003200
6	-2.3065020	-0.5748460	0.0000150	6	-2.3219820	-0.5951750	0.0002900	6	-2.3310860	-0.5886280	0.0001550
8	1.1236850	-1.3892690	-0.0000280	8	1.1635440	-1.3753970	-0.0003360	8	1.1595060	-1.3799980	-0.0001290
1	2.8085010	-0.2659230	0.0001020	1	2.8058990	-0.2490850	0.0008100	1	2.8072580	-0.2567090	0.0005300
1	1.6855050	1.8560540	0.0000170	1	1.6634380	1.8503450	0.0005170	1	1.6695240	1.8487180	-0.0000470
1	-2.7278310	-0.9561020	-0.9271160	1	-2.7359220	-0.9707580	-0.9213430	1	-2.7511390	-0.9617730	-0.9192580
1	-2.7281040	-0.9557420	0.9271710	1	-2.7364080	-0.9690710	0.9223920	1	-2.7507420	-0.9612290	0.9199670
1	-0.6896490	2.2224950	-0.0001550	1	-0.6927790	2.2142990	-0.0010370	1	-0.6842830	2.2152550	-0.0001470
	M12 CBS-QB3				M12 CBS-APNO				M12 G3		
6	0.7508650	0.8407160	0.0000020	6	-0.7591190	0.8340430	0.0000020	6	0.7604260	0.8355370	0.0000000
6	-0.6449070	1.0584230	-0.0000030	6	0.6365160	1.0699380	-0.0000010	6	-0.6353040	1.0749530	-0.0000010
6	1.3829680	-0.4580290	-0.0000050	6	-1.3752070	-0.4689330	0.0000020	6	1.3704700	-0.4687950	-0.0000020
6	-1.6002290	0.1182860	-0.0000010	6	1.6007170	0.1269170	-0.0000010	6	-1.6020690	0.1304510	0.0000000
6	-2.5497260	-0.7655430	0.0000030	6	2.5481490	-0.7686170	0.0000000	6	-2.5473990	-0.7723120	0.0000010
8	2.5957660	-0.6134040	0.0000040	8	-2.5791350	-0.6106810	-0.0000020	8	2.5806450	-0.6147030	0.0000020
1	0.6996370	-1.3304920	-0.0000200	1	-0.7209560	-1.3398310	0.0000070	1	0.7171600	-1.3378110	-0.0000080
1	1.4160230	1.6970750	0.0000130	1	-1.4276680	1.6760630	0.0000000	1	1.4306000	1.6755570	0.0000040
1	-2.9646500	-1.1573080	-0.9266060	1	2.9554100	-1.1538250	0.9213970	1	-2.9549730	-1.1608810	-0.9191830

Table 11: Cartesian coordinates for minima (M10–M16) on the C_5H_5O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-2.9646550	-1.1572930	0.9266170	1	2.9554060	-1.1538310	-0.9213970	1	-2.9549730	-1.1608800	0.9191850
1	-0.9863070	2.0921320	-0.0000070	1	0.9645480	2.0967820	-0.0000010	1	-0.9597170	2.1026410	-0.0000020
	M13 CBS-QB3				M13 CBS-APNO				M13 G3		
6	0.8084350	0.9761030	-0.0002270	6	0.8261090	0.9746950	-0.0002540	6	-0.8228150	0.9790970	0.0003050
6	-0.6180350	0.8355780	-0.0000100	6	-0.6119170	0.8343820	0.0000520	6	0.6145460	0.8351330	-0.0000440
6	1.6990600	-0.0120340	0.0007130	6	1.6977400	-0.0182690	0.0001690	6	-1.6984950	-0.0152440	-0.0003110
6	-1.3265630	-0.3788430	0.0001040	6	-1.3145360	-0.3813990	-0.0001890	6	1.3154610	-0.3830680	0.0002360
6	-2.6875460	-0.4937010	-0.0000710	6	-2.6888880	-0.4818240	0.0001000	6	2.6912420	-0.4851190	-0.0001280
8	2.4893550	-0.8640170	-0.0003670	8	2.4595140	-0.8657760	0.0000790	8	-2.4682570	-0.8680170	-0.0000450
1	-0.7437290	-1.2996580	0.0003770	1	-0.7452840	-1.2988140	-0.0006200	1	0.7443960	-1.2987090	0.0007640
1	1.2542730	1.9654780	-0.0000800	1	1.2764010	1.9502780	-0.0001730	1	-1.2684420	1.9569800	0.0002950
1	-3.3274660	0.3821230	-0.0003820	1	-3.3137920	0.3944240	0.0005240	1	3.3179110	0.3891730	-0.0006460
1	-3.1710920	-1.4617510	0.0000690	1	-3.1759890	-1.4392990	-0.0001040	1	3.1793990	-1.4415590	0.0001140
1	-1.1789340	1.7633300	-0.0001030	1	-1.1684970	1.7541130	0.0004700	1	1.1731500	1.7534660	-0.0005200
	M14 CBS-QB3										
6	-0.7524310	0.8180140	-0.0000060								
6	0.5965560	0.7823360	-0.0000240								
6	-1.5707220	-0.3969840	-0.0000030								
6	1.4159970	-0.4136160	-0.0000160								
6	2.7537090	-0.3738060	0.0000770								
8	-2.7552170	-0.4895590	-0.0000430								
1	0.8944500	-1.3652250	-0.0000210								
1	-1.2846510	1.7680530	-0.0000390								
1	3.2938760	0.5677790	0.0001400								
1	3.3481710	-1.2792960	0.0001920								
1	1.1312430	1.7294960	-0.0000920								
	M15 CBS-QB3				M15 CBS-APNO				M15 G3		
6	0.5821270	1.1031570	-0.0000600	6	-0.6140650	1.0959450	0.0003460	6	-0.6094410	1.1022370	0.0002090
6	-0.8497870	1.1072100	0.0001670	6	0.8310510	1.1124850	-0.0001060	6	0.8356580	1.1127720	-0.0001370
6	1.4148130	0.0660920	-0.0001530	6	-1.4237550	0.0530870	0.0000520	6	-1.4229350	0.0578930	0.0000290
6	-1.7274950	0.0056730	0.0002530	6	1.7276740	0.0303580	-0.0002650	6	1.7290380	0.0261670	-0.0002500
6	-1.4139900	-1.3244250	0.0000660	6	1.4346210	-1.3172480	0.0001560	6	1.4315930	-1.3219360	0.0001350
8	2.1901550	-0.7990160	-0.0002650	8	-2.1592370	-0.8166780	-0.0001750	8	-2.1667480	-0.8172000	-0.0000380
1	-2.7829990	0.2656040	0.0004930	1	2.7699800	0.3032440	-0.0007600	1	2.7721100	0.2946160	-0.0006760

Table 11: Cartesian coordinates for minima (M10–M16) on the C_5H_5O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	1.1076320	2.0539120	-0.0002440	1	-1.1457540	2.0308100	0.0007280	1	-1.1355280	2.0402500	0.0007610
1	-0.3957960	-1.6943850	-0.0002120	1	0.4330930	-1.7055680	0.0007360	1	0.4296310	-1.7076320	0.0006540
1	-2.1934730	-2.0754300	0.0001730	1	2.2278550	-2.0420610	-0.0000410	1	2.2208240	-2.0504140	-0.0000330
1	-1.2906100	2.0961900	0.0002720	1	1.2555650	2.0992340	-0.0003510	1	1.2634730	2.0979820	-0.0003160
	M16 CBS-QB3				M16 CBS-APNO				M16 G3		
6	0.0508700	1.1958500	-0.0000240	6	0.0489500	1.1958930	-0.0000540	6	0.0481890	1.1963190	-0.0000530
6	1.3786630	0.7524340	-0.0002170	6	1.3773760	0.7515260	-0.0001520	6	1.3783260	0.7531590	-0.0001630
6	-0.8460370	0.0426790	0.0001160	6	-0.8402900	0.0378080	0.0001050	6	-0.8385310	0.0378510	0.0000770
6	1.4414030	-0.6304100	-0.0000500	6	1.4340840	-0.6357750	-0.0001450	6	1.4358800	-0.6352450	-0.0001430
6	0.0596540	-1.2072060	-0.0000050	6	0.0426520	-1.2086610	0.0000490	6	0.0442550	-1.2099470	0.0000470
8	-2.0638150	0.0408940	0.0001950	8	-2.0392940	0.0502240	0.0001930	8	-2.0437070	0.0496640	0.0002180
1	2.3516130	-1.2148340	-0.0001710	1	2.3326680	-1.2217860	-0.0002460	1	2.3337140	-1.2220240	-0.0002250
1	-0.2936610	2.2205110	-0.0000270	1	-0.2957250	2.2114640	-0.0000630	1	-0.2973240	2.2112480	-0.0000510
1	-0.1498910	-1.8277050	-0.8784900	1	-0.1681520	-1.8158930	-0.8756980	1	-0.1662080	-1.8187580	-0.8745220
1	-0.1497250	-1.8275990	0.8785970	1	-0.1679420	-1.8157990	0.8759140	1	-0.1660100	-1.8186610	0.8747330
1	2.2448560	1.4023870	-0.0003820	1	2.2368650	1.3954780	-0.0002620	1	2.2367720	1.3980570	-0.0002680

Table 12: Cartesian coordinates for minima (M17–M27) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M17 CBS-QB3				M17 CBS-APNO				M17 G3		
6	0.694148	0.063394	0.463505	6	0.690391	0.049158	0.463494	6	0.691269	0.049414	0.466486
6	-0.247967	1.196513	0.172534	6	-0.250048	1.190761	0.171930	6	-0.250555	1.191043	0.176299
6	-1.352862	-0.725611	-0.166626	6	-1.341770	-0.730710	-0.165511	6	-1.341800	-0.730899	-0.168059
8	-0.110917	-1.132565	0.214200	8	-0.099322	-1.113380	0.212620	8	-0.098253	-1.114474	0.216589
1	0.013679	2.240029	0.258207	1	0.009082	2.227102	0.259276	1	0.009801	2.227130	0.262696
6	1.955091	0.002605	-0.397924	6	1.944226	0.009632	-0.396748	6	1.941763	0.010488	-0.400686
1	2.523542	-0.904113	-0.178365	1	2.519467	-0.884164	-0.180159	1	2.519632	-0.881964	-0.188011
1	1.690370	0.007862	-1.457269	1	1.681198	0.007103	-1.449239	1	1.673079	0.007441	-1.451046
1	2.589436	0.869178	-0.191637	1	2.565750	0.877797	-0.194977	1	2.564656	0.878081	-0.204111
6	-1.464414	0.653252	-0.203676	6	-1.468963	0.645503	-0.203775	6	-1.468911	0.645870	-0.205870
1	-2.356697	1.192835	-0.485870	1	-2.358415	1.175280	-0.480869	1	-2.356732	1.177065	-0.485829
1	-2.059750	-1.508351	-0.390535	1	-2.039259	-1.510374	-0.385594	1	-2.035068	-1.513442	-0.390189
1	0.982784	0.022163	1.524994	1	0.973743	0.028224	1.514262	1	0.980070	0.025979	1.514758
	M18 CBS-QB3				M18 CBS-APNO				M18 G3		
6	1.726596	-0.103753	0.000004	6	1.745185	-0.129551	-0.000046	6	1.746193	-0.128608	-0.000031
6	0.882559	1.075962	0.000014	6	0.912605	1.057046	-0.000078	6	0.915576	1.057033	-0.000049
6	-0.514366	1.260337	-0.000008	6	-0.487674	1.259043	0.000050	6	-0.485219	1.260663	0.000033
6	-1.593123	0.401671	-0.000008	6	-1.590851	0.426368	0.000066	6	-1.591012	0.428784	0.000043
8	1.392001	-1.280607	-0.000015	8	1.386686	-1.281279	0.000127	8	1.382886	-1.286068	0.000083
1	1.459353	1.997601	0.000029	1	1.490836	1.966710	-0.000162	1	1.494104	1.965867	-0.000105
1	-0.795583	2.311650	-0.000024	1	-0.743279	2.307012	0.000135	1	-0.738813	2.308512	0.000087
6	-1.655861	-1.084952	0.000016	6	-1.712562	-1.067134	-0.000101	6	-1.714417	-1.065314	-0.000065
1	-2.223257	-1.428926	0.874816	1	-2.279645	-1.383946	0.873283	1	-2.280843	-1.384673	0.872330
1	-2.223097	-1.428957	-0.874878	1	-2.280339	-1.383682	-0.873127	1	-2.281252	-1.384503	-0.872255
1	-0.673964	-1.548787	0.000097	1	-0.762304	-1.570100	-0.000526	1	-0.764172	-1.568364	-0.000320
1	-2.561640	0.898470	-0.000032	1	-2.534557	0.949598	0.000221	1	-2.534044	0.951673	0.000139
1	2.807344	0.148214	0.000011	1	2.815580	0.090003	-0.000182	1	2.815202	0.084684	-0.000122
	M19 CBS-QB3				M19 CBS-APNO				M19 G3		
6	-1.362396	-0.397532	0.000000	6	-1.358266	-0.406627	0.000000	6	1.355693	-0.406355	0.000000
6	-0.686288	0.884432	0.000000	6	-0.700845	0.878312	0.000000	6	0.701486	0.878323	0.000000
6	0.686260	1.171020	0.000000	6	0.676136	1.176077	0.000000	6	-0.676560	1.177171	0.000000
6	1.791626	0.342982	0.000000	6	1.790364	0.351842	0.000000	6	-1.791673	0.352170	0.000000
8	-2.582817	-0.489620	0.000000	8	-2.569306	-0.491702	0.000000	8	2.573434	-0.492179	0.000000

Table 12: Cartesian coordinates for minima (M17–M27) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-1.373234	1.725857	0.000000	1	-1.384630	1.709802	0.000000	1	1.385009	1.709222	0.000000
1	0.918794	2.233304	0.000000	1	0.896492	2.231057	0.000000	1	-0.896330	2.231787	0.000000
6	1.833733	-1.153485	0.000000	6	1.839773	-1.152210	0.000000	6	-1.840792	-1.152410	0.000000
1	2.863516	-1.513267	0.000001	1	2.868579	-1.491547	0.000001	1	-2.868867	-1.493478	-0.000001
1	1.333157	-1.574054	0.879402	1	1.356341	-1.572125	0.877985	1	-1.357869	-1.573616	-0.877193
1	1.333157	-1.574055	-0.879401	1	1.356342	-1.572125	-0.877985	1	-1.357870	-1.573616	0.877193
1	2.753713	0.846176	0.000000	1	2.740701	0.857579	0.000000	1	-2.742377	0.856029	0.000000
1	-0.744176	-1.311502	0.000000	1	-0.762348	-1.313385	0.000000	1	0.761903	-1.312285	0.000000
	M20 CBS-QB3				M20 CBS-APNO						
6	-1.607064	-0.402419	0.058716	6	-1.620222	-0.401056	0.064440				
6	-0.835404	0.833152	-0.133135	6	-0.829677	0.832191	-0.134320				
6	0.483614	0.901161	0.099296	6	0.477739	0.896573	0.096338				
6	1.371438	-0.208974	0.568996	6	1.379328	-0.204436	0.576015				
8	-2.771572	-0.573980	-0.097690	8	-2.756726	-0.573330	-0.098897				
1	-1.391173	1.704279	-0.478869	1	-1.378017	1.692472	-0.482440				
1	0.976203	1.856661	-0.076517	1	0.962717	1.844383	-0.084457				
6	2.517468	-0.495020	-0.417042	6	2.505280	-0.496523	-0.421884				
1	3.128884	0.395649	-0.589011	1	3.103896	0.389882	-0.612654				
1	3.170812	-1.278836	-0.027009	1	3.164240	-1.266503	-0.034557				
1	2.128173	-0.827631	-1.382275	1	2.103845	-0.840939	-1.369651				
1	1.801318	0.083943	1.535573	1	1.814845	0.109777	1.522568				
1	0.778033	-1.109624	0.738644	1	0.807595	-1.102924	0.768829				
	M21 CBS-QB3				M21 CBS-APNO				M21 G3		
6	-1.953476	-0.023528	0.000008	6	-1.973461	-0.014542	0.000003	6	-1.974875	-0.011758	0.000003
6	-0.974808	1.046139	-0.000182	6	-0.974731	1.034202	-0.000182	6	-0.977059	1.035043	-0.000188
6	0.423110	0.909204	-0.000161	6	0.428271	0.887592	-0.000157	6	0.426729	0.887746	-0.000162
6	1.130817	-0.269360	0.000044	6	1.147810	-0.287532	0.000047	6	1.147879	-0.288423	0.000052
8	-1.711650	-1.223995	0.000218	8	-1.749153	-1.201215	0.000214	8	-1.747169	-1.204969	0.000222
1	-1.384144	2.052012	-0.000358	1	-1.365329	2.037871	-0.000358	1	-1.366560	2.038741	-0.000371
1	0.995686	1.835678	-0.000326	1	0.987841	1.810286	-0.000320	1	0.986112	1.809897	-0.000330
1	-3.006934	0.325108	-0.000051	1	-3.008614	0.334852	-0.000059	1	-3.009235	0.332159	-0.000060
6	2.619286	-0.342267	0.000056	6	2.646473	-0.333120	0.000058	6	2.647537	-0.331726	0.000058
1	2.981289	-0.894776	0.875862	1	3.015191	-0.865174	0.874136	1	3.019875	-0.861826	0.873295
1	2.981288	-0.895130	-0.875526	1	3.015193	-0.865540	-0.873795	1	3.019874	-0.862144	-0.872986

Table 12: Cartesian coordinates for minima (M17–M27) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	3.083658	0.646574	-0.000142	1	3.081479	0.660750	-0.000149	1	3.081375	0.662476	-0.000123
1	0.572788	-1.198634	0.000208	1	0.621295	-1.222922	0.000212	1	0.624642	-1.224842	0.000223
	M22 CBS-QB3				M22 CBS-APNO				M22 G3		
6	-1.701467	-0.405909	-0.000059	6	-1.701115	-0.413821	-0.000050	6	-1.700169	-0.414677	-0.000051
6	-0.831706	0.750007	-0.000020	6	-0.841276	0.744298	-0.000025	6	-0.842097	0.742824	-0.000024
6	0.572561	0.739602	0.000012	6	0.568596	0.739123	0.000015	6	0.568880	0.738858	0.000015
6	1.404223	-0.355677	0.000053	6	1.402759	-0.360400	0.000042	6	1.404928	-0.361073	0.000043
8	-2.921276	-0.324965	-0.000076	8	-2.908945	-0.317101	-0.000083	8	-2.914709	-0.315499	-0.000083
1	-1.348789	1.704149	-0.000021	1	-1.354729	1.689775	-0.000039	1	-1.355092	1.687948	-0.000037
1	1.055169	1.715488	0.000009	1	1.039376	1.709369	0.000025	1	1.039062	1.708772	0.000024
1	-1.213989	-1.401465	-0.000083	1	-1.242780	-1.401984	-0.000040	1	-1.246365	-1.402591	-0.000045
6	2.893846	-0.272702	0.000078	6	2.899810	-0.267663	0.000084	6	2.902713	-0.266838	0.000084
1	3.315945	-0.778992	0.876823	1	3.318419	-0.760210	0.874674	1	3.323915	-0.757660	0.873859
1	3.315975	-0.779021	-0.876637	1	3.318468	-0.760220	-0.874478	1	3.323962	-0.757673	-0.873662
1	3.244566	0.761507	0.000066	1	3.235280	0.763609	0.000087	1	3.237662	0.764394	0.000085
1	0.976596	-1.353871	0.000070	1	0.984882	-1.352758	0.000034	1	0.988995	-1.353762	0.000038
	M23 CBS-QB3				M23 CBS-APNO				M23 G3		
6	-1.936611	0.544046	0.000082	6	-1.940558	0.544370	-0.000079	6	-1.939663	0.548146	-0.000090
6	-0.486302	0.583157	0.000083	6	-0.494620	0.573280	0.000002	6	-0.495554	0.575588	-0.000007
6	0.276098	-0.590553	0.000041	6	0.275252	-0.603115	-0.000015	6	0.273734	-0.602362	-0.000021
6	1.647267	-0.683398	0.000052	6	1.651876	-0.684002	0.000047	6	1.652018	-0.685172	0.000047
8	-2.603201	-0.481603	-0.000341	8	-2.598198	-0.471513	-0.000160	8	-2.599411	-0.474669	-0.000142
1	-0.016464	1.561068	0.000127	1	-0.028266	1.541889	0.000078	1	-0.026894	1.542754	0.000071
1	-0.296893	-1.513472	0.000005	1	-0.277487	-1.526174	-0.000079	1	-0.279270	-1.524717	-0.000087
6	2.628566	0.441901	0.000126	6	2.632181	0.452607	0.000158	6	2.634090	0.450923	0.000160
1	3.283970	0.379142	0.876994	1	3.275834	0.396274	0.874770	1	3.278437	0.396713	0.873929
1	3.284523	0.378780	-0.876296	1	3.276523	0.395833	-0.873913	1	3.279139	0.396262	-0.873057
1	2.157174	1.424713	-0.000217	1	2.155412	1.424246	-0.000278	1	2.158648	1.423060	-0.000284
1	2.075784	-1.682210	0.000037	1	2.081924	-1.672140	0.000059	1	2.082339	-1.672558	0.000060
1	-2.436597	1.533880	-0.000228	1	-2.443146	1.513343	-0.000038	1	-2.444857	1.513109	-0.000026
	M24 CBS-QB3				M24 CBS-APNO				M24 G3		
6	1.915903	0.478725	0.000217	6	1.915226	0.471064	0.000076	6	1.914635	0.474571	0.000039
6	0.414878	0.674455	0.000358	6	0.419555	0.671708	0.000156	6	0.418330	0.674913	0.000162
6	-0.378043	-0.591705	0.000269	6	-0.375409	-0.601273	0.000129	6	-0.373105	-0.601190	0.000134

Table 12: Cartesian coordinates for minima (M17–M27) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	-1.767186	-0.646929	-0.000078	6	-1.768776	-0.649802	-0.000091	6	-1.767449	-0.651492	-0.000088
8	2.476453	-0.586450	-0.000296	8	2.466710	-0.573805	0.000046	8	2.466893	-0.576586	0.000050
1	0.176924	1.311729	-0.866748	1	0.186292	1.292948	-0.865903	1	0.181132	1.295649	-0.864853
1	0.194366	-1.511263	0.000490	1	0.181058	-1.519310	0.000310	1	0.185027	-1.517829	0.000319
6	-2.630816	0.428706	-0.000388	6	-2.625810	0.440815	-0.000312	6	-2.626632	0.438957	-0.000309
1	-2.276086	1.452817	-0.000376	1	-2.264426	1.453660	-0.000328	1	-2.267551	1.452077	-0.000322
1	-3.703344	0.283025	-0.000671	1	-3.691403	0.302435	-0.000474	1	-3.691958	0.301993	-0.000475
1	-2.209324	-1.640373	-0.000116	1	-2.215676	-1.630646	-0.000082	1	-2.213774	-1.632246	-0.000081
1	2.500314	1.424662	-0.000176	1	2.495372	1.403436	0.000042	1	2.496036	1.402968	0.000068
1	0.177109	1.311488	0.867699	1	0.186386	1.292845	0.866319	1	0.181274	1.295517	0.865317
	M25 CBS-QB3				M25 CBS-APNO				M25 G3		
6	1.554961	-0.106496	-0.305356	6	1.520630	-0.093199	-0.354365	6	1.504298	-0.091369	-0.363666
6	0.584749	-0.871568	0.589720	6	0.570490	-0.835555	0.561717	6	0.570474	-0.859317	0.547743
6	-0.717329	-1.103779	-0.126930	6	-0.766515	-1.092466	-0.090720	6	-0.778335	-1.097497	-0.089087
6	-1.711245	-0.138668	-0.270081	6	-1.761380	-0.126942	-0.244165	6	-1.758017	-0.114106	-0.236513
8	1.884119	1.036644	-0.123586	8	2.058298	0.921323	-0.073895	8	2.048164	0.920341	-0.060898
1	0.448564	-0.290521	1.505364	1	0.473771	-0.265805	1.478409	1	0.488931	-0.312417	1.479767
1	-0.875329	-2.076258	-0.579746	1	-0.956911	-2.081237	-0.469473	1	-0.987732	-2.084579	-0.460803
6	-1.663693	1.160460	0.190719	6	-1.683440	1.198648	0.160841	6	-1.651127	1.212313	0.163288
1	-0.792392	1.560497	0.694379	1	-0.804491	1.605202	0.626722	1	-0.761034	1.604081	0.619206
1	-2.497248	1.833172	0.034515	1	-2.510118	1.866320	0.001878	1	-2.465015	1.896305	0.011078
1	-2.610086	-0.450413	-0.797206	1	-2.673628	-0.447370	-0.720911	1	-2.680537	-0.418812	-0.702744
1	1.927349	-0.676311	-1.184126	1	1.689492	-0.563569	-1.332031	1	1.657830	-0.530919	-1.354694
1	1.041532	-1.833007	0.847073	1	1.036799	-1.787043	0.806720	1	1.038495	-1.816528	0.764795
	M26 CBS-QB3				M26 CBS-APNO				M26 G3		
6	-1.616681	0.007683	0.121307	6	-1.623473	0.031808	0.159440	6	-1.623094	0.027820	0.157885
6	-0.792690	1.097151	0.208097	6	-0.772057	1.089344	0.228276	6	-0.775851	1.091589	0.227530
6	0.579264	1.226623	-0.122275	6	0.602680	1.198163	-0.166291	6	0.599452	1.203088	-0.162608
6	1.588218	0.226847	-0.211644	6	1.622279	0.210994	-0.206369	6	1.618100	0.213091	-0.208322
8	-1.319315	-1.227307	-0.323796	8	-1.381375	-1.189936	-0.345734	8	-1.371425	-1.195172	-0.346572
1	-1.308023	2.012742	0.482567	1	-1.235724	2.004531	0.555825	1	-1.243508	2.006101	0.550534
1	0.911393	2.239485	-0.330844	1	0.919884	2.193994	-0.427862	1	0.916756	2.199038	-0.422747
6	1.610125	-1.014487	0.355830	6	1.623833	-1.035510	0.375820	6	1.621467	-1.033141	0.377437
1	2.460879	-1.668935	0.213313	1	2.488881	-1.668045	0.292288	1	2.482218	-1.670053	0.288479

Table 12: Cartesian coordinates for minima (M17–M27) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	0.841818	-1.358627	1.038438	1	0.804285	-1.400472	0.966363	1	0.809284	-1.392269	0.980699
1	-0.376466	-1.280765	-0.548418	1	-0.543078	-1.217235	-0.774090	1	-0.521073	-1.218573	-0.765202
1	2.479410	0.525832	-0.760641	1	2.531750	0.515842	-0.699146	1	2.523759	0.513896	-0.709685
1	-2.663906	0.085824	0.388063	1	-2.634574	0.122076	0.507233	1	-2.636478	0.108553	0.498966
	M27 CBS-QB3				M27 CBS-APNO				M27 G3		
6	0.782089	0.002682	0.443721	6	0.784309	-0.008014	0.434208	6	0.784970	-0.008684	0.435124
6	-0.120199	-1.186992	0.236486	6	-0.130027	-1.190319	0.213637	6	-0.130378	-1.191075	0.215695
6	-1.388179	-0.777402	-0.150607	6	-1.403052	-0.765980	-0.146259	6	-1.403851	-0.766519	-0.146683
6	-1.475193	0.607567	-0.203118	6	-1.469100	0.623876	-0.188319	6	-1.469027	0.624396	-0.190107
8	1.950993	-0.030747	-0.385432	8	1.938320	-0.045563	-0.367616	8	1.938565	-0.046172	-0.369547
1	0.218592	-2.207260	0.357752	1	0.195051	-2.208165	0.322010	1	0.194726	-2.208585	0.324885
1	-2.207144	-1.449235	-0.379672	1	-2.227799	-1.421063	-0.360803	1	-2.228114	-1.421524	-0.362298
6	-0.153953	1.223036	0.169901	6	-0.127512	1.218966	0.162064	6	-0.127949	1.219835	0.164293
1	-0.241922	1.876703	1.045688	1	-0.192099	1.872351	1.028016	1	-0.192814	1.870998	1.031705
1	0.271642	1.839578	-0.630421	1	0.284902	1.814134	-0.648870	1	0.286390	1.818501	-0.642707
1	1.656003	-0.238514	-1.279399	1	1.684591	-0.174457	-1.264999	1	1.680187	-0.171220	-1.273251
1	-2.358169	1.173736	-0.468515	1	-2.339906	1.201029	-0.436054	1	-2.337911	1.203171	-0.439846
1	1.185667	0.037623	1.459724	1	1.160998	0.009505	1.449633	1	1.166427	0.010313	1.447956

Table 13: Cartesian coordinates for minima (M28–M35) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M28 CBS-QB3				M28 CBS-APNO				M28 G3		
6	-0.676700	0.052177	-0.231132	6	-0.672554	0.045880	-0.281354	6	-0.673156	0.047103	-0.282951
6	0.243995	1.226897	-0.040132	6	0.242515	1.227290	-0.051000	6	0.244811	1.228336	-0.054865
6	1.368914	-0.783457	0.053404	6	1.349728	-0.776044	0.062854	6	1.350172	-0.778038	0.064893
8	0.043188	-1.130443	-0.064627	8	0.045118	-1.118901	-0.080989	8	0.044024	-1.120334	-0.086055
1	0.194864	1.945397	-0.871091	1	0.213140	1.933094	-0.878352	1	0.221042	1.929644	-0.886418
6	-2.120132	-0.023611	0.099908	6	-2.104398	-0.024237	0.125608	6	-2.104799	-0.023320	0.129540
1	-2.561227	-0.940599	-0.298738	1	-2.575729	-0.908049	-0.290029	1	-2.577420	-0.907976	-0.282048
1	-2.301318	-0.016851	1.188691	1	-2.205273	-0.068678	1.211588	1	-2.206218	-0.064273	1.214567
1	-2.657473	0.827868	-0.325474	1	-2.640147	0.850973	-0.227019	1	-2.643618	0.849066	-0.224233
6	1.581247	0.531113	0.065402	6	1.570175	0.521102	0.084722	6	1.570454	0.520651	0.089777
1	2.540336	1.017560	0.153099	1	2.525552	0.992234	0.194812	1	2.523894	0.995093	0.203289
1	2.051083	-1.617531	0.115548	1	2.032481	-1.597388	0.141589	1	2.028730	-1.602133	0.145311
1	0.004287	1.808989	0.870281	1	-0.023760	1.785078	0.850344	1	-0.023495	1.794868	0.839612
	M29 CBS-QB3				M29 CBS-APNO				M29 G3		
6	0.793325	0.181622	-0.031208	6	0.802679	0.187293	-0.052225	6	0.801326	0.184902	-0.050540
6	-0.208657	-0.966492	-0.076408	6	-0.211858	-0.941552	-0.116216	6	-0.211410	-0.946786	-0.110115
6	-1.667507	-0.599221	0.019711	6	-1.673054	-0.589248	-0.013616	6	-1.672959	-0.591067	-0.017931
6	-2.182913	0.602353	0.066487	6	-2.209979	0.606656	0.174977	6	-2.206811	0.609788	0.176357
8	0.466914	1.342885	-0.072598	8	0.515237	1.331090	-0.161806	8	0.509411	1.333132	-0.161741
1	-0.024850	-1.516517	-1.011291	1	-0.032280	-1.461364	-1.058277	1	-0.027947	-1.478207	-1.044629
1	-2.341135	-1.464768	0.047598	1	-2.340327	-1.439475	-0.098480	1	-2.339409	-1.439717	-0.112890
1	0.053599	-1.683394	0.713389	1	0.040408	-1.668135	0.654676	1	0.036694	-1.666369	0.668658
6	2.252895	-0.231025	0.077685	6	2.238099	-0.251620	0.153314	6	2.240133	-0.247671	0.150198
1	2.490904	-1.055125	-0.600311	1	2.486178	-1.099565	-0.477644	1	2.502784	-1.066291	-0.512588
1	2.890996	0.625883	-0.133750	1	2.903437	0.574500	-0.056109	1	2.898924	0.591519	-0.024001
1	2.454653	-0.580340	1.096061	1	2.370672	-0.562399	1.186698	1	2.375181	-0.599184	1.169562
1	-3.182342	1.007758	0.131481	1	-3.225302	0.938554	0.266177	1	-3.223188	0.938197	0.261998
	M30 CBS-QB3				M30 CBS-APNO				M30 G3		
6	-1.292050	1.207644	0.381865	6	-1.395692	1.156076	0.322749	6	-1.391202	1.161340	0.314752
6	-0.875782	-0.194859	-0.017768	6	-0.856020	-0.214350	-0.021467	6	-0.854749	-0.214156	-0.016809
6	0.345428	-0.784004	0.690204	6	0.350145	-0.700746	0.767974	6	0.351015	-0.697456	0.775204
6	1.670914	-0.205655	0.234506	6	1.663277	-0.110932	0.301102	6	1.661855	-0.100469	0.308001
6	1.868858	0.645439	-0.737132	6	1.854201	0.578662	-0.812474	6	1.851243	0.559691	-0.828606

Table 13: Cartesian coordinates for minima (M28–M35) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.698546	1.144884	-1.212852	1	2.704248	1.033097	-1.279586	1	2.701935	1.013273	-1.294368
1	2.541323	-0.578131	0.788453	1	2.515192	-0.309021	0.939873	1	2.507562	-0.265489	0.962663
1	0.251784	-0.630803	1.772999	1	0.213931	-0.457971	1.819813	1	0.212009	-0.456988	1.826836
1	0.340966	-1.862683	0.509106	1	0.388373	-1.781264	0.679891	1	0.392016	-1.777913	0.688460
8	-1.492080	-0.840688	-0.831949	8	-1.363865	-0.898507	-0.846568	8	-1.366638	-0.905831	-0.840979
1	-2.046609	1.576560	-0.311472	1	-2.085216	1.479529	-0.444855	1	-2.093810	1.471901	-0.446033
1	-0.435750	1.884867	0.407936	1	-0.596222	1.878742	0.439074	1	-0.591516	1.887519	0.402400
1	-1.717825	1.179421	1.391376	1	-1.924859	1.092682	1.271032	1	-1.904068	1.120636	1.272631
	M31 CBS-QB3				M31 CBS-APNO				M31 G3		
6	-0.810081	0.155222	0.195651	6	-0.805094	0.157059	0.193809	6	-0.805504	0.157735	0.193669
6	0.403130	-0.342620	0.976807	6	0.399344	-0.363722	0.960900	6	0.396488	-0.374815	0.957032
6	1.675907	-0.353614	0.124456	6	1.659238	-0.395053	0.105355	6	1.644551	-0.430009	0.083297
6	1.909090	0.388260	-0.926020	6	1.928053	0.428732	-0.897626	6	1.950424	0.448787	-0.866840
8	-1.133642	1.320148	0.216826	8	-1.116592	1.301507	0.242665	8	-1.103875	1.311322	0.241274
1	0.551506	0.316959	1.836672	1	0.556138	0.279517	1.820201	1	0.568893	0.273501	1.809125
1	2.448878	-1.041823	0.468957	1	2.396243	-1.134673	0.377602	1	2.332962	-1.234318	0.286910
1	0.226564	-1.356573	1.350010	1	0.199196	-1.368002	1.322331	1	0.185273	-1.371669	1.330707
6	-1.564875	-0.879963	-0.615305	6	-1.573564	-0.848542	-0.632853	6	-1.586191	-0.837651	-0.634989
1	-2.092852	-1.559303	0.062913	1	-2.110801	-1.519478	0.033154	1	-2.110685	-1.525875	0.022635
1	-2.288633	-0.387241	-1.263058	1	-2.281111	-0.336159	-1.270011	1	-2.305807	-0.317569	-1.251742
1	-0.875887	-1.487004	-1.208798	1	-0.898329	-1.451604	-1.231026	1	-0.920237	-1.425839	-1.257700
1	1.420534	1.150086	-1.514834	1	1.423538	1.247491	-1.371077	1	1.481989	1.326912	-1.263145
	M32 CBS-QB3				M32 CBS-APNO				M32 G3		
6	1.352368	1.100790	-0.604133	6	1.448612	1.044383	-0.597807	6	1.423157	1.062071	-0.595734
6	0.933066	-0.143772	-0.023383	6	0.926086	-0.152113	-0.013265	6	0.927255	-0.147792	-0.019506
6	-0.269986	-0.855978	-0.634848	6	-0.272713	-0.832072	-0.647372	6	-0.272119	-0.839492	-0.640871
6	-1.605347	-0.244959	-0.278814	6	-1.609704	-0.227172	-0.285529	6	-1.610531	-0.236104	-0.278468
6	-1.832587	0.659850	0.668959	6	-1.843502	0.686879	0.634321	6	-1.844398	0.682634	0.638167
1	-2.834378	1.026054	0.861324	1	-2.843653	1.036713	0.819999	1	-2.843559	1.032507	0.826203
1	-2.445608	-0.617742	-0.860721	1	-2.442620	-0.621048	-0.847135	1	-2.442590	-0.634499	-0.836729
1	-0.168667	-0.871424	-1.727295	1	-0.167956	-0.816002	-1.729896	1	-0.171423	-0.835383	-1.723776
1	-0.240060	-1.897482	-0.299086	1	-0.259947	-1.873848	-0.342672	1	-0.252109	-1.878437	-0.327508
8	1.527886	-0.618676	0.947788	8	1.447459	-0.620122	0.990868	8	1.474985	-0.622325	0.975312
1	2.207365	1.607755	-0.174467	1	2.296636	1.516307	-0.137491	1	2.271885	1.541549	-0.146525

Table 13: Cartesian coordinates for minima (M28–M35) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-1.041019	1.058053	1.294758	1	-1.063706	1.113324	1.241152	1	-1.066134	1.115365	1.241297
1	0.834195	1.548605	-1.443499	1	1.008900	1.486104	-1.472988	1	0.963875	1.509602	-1.456989
	M33 CBS-QB3				M33 CBS-APNO				M33 G3		
6	-1.695044	1.095574	-0.222748	6	-1.790063	1.022731	-0.218694	6	-1.781662	1.028163	-0.223280
6	-1.042954	-0.154402	0.058659	6	-1.035861	-0.160669	0.068177	6	-1.035451	-0.156621	0.069148
6	0.282368	-0.135251	0.832278	6	0.280852	-0.050247	0.823719	6	0.280945	-0.055353	0.826853
6	1.402217	0.488347	0.039774	6	1.389986	0.500640	-0.037997	6	1.392868	0.501349	-0.028889
6	2.459921	-0.173346	-0.418931	6	2.479253	-0.161872	-0.367801	6	2.475610	-0.165191	-0.375346
1	3.234166	0.324323	-0.991620	1	3.238491	0.282799	-0.986979	1	3.237594	0.281349	-0.988814
1	1.312762	1.552704	-0.169579	1	1.259820	1.509185	-0.400630	1	1.269146	1.516902	-0.371367
1	0.135444	0.423815	1.765158	1	0.142106	0.596814	1.687497	1	0.142729	0.580607	1.698914
1	0.518648	-1.169591	1.085054	1	0.537775	-1.039630	1.178958	1	0.535933	-1.048453	1.173118
8	-1.538845	-1.218181	-0.314829	8	-1.450203	-1.250904	-0.298057	8	-1.458585	-1.250727	-0.297839
1	-2.622434	1.077709	-0.781296	1	-2.706288	0.929594	-0.771217	1	-2.696596	0.941796	-0.777497
1	2.590169	-1.235223	-0.235781	1	2.653035	-1.170751	-0.033146	1	2.643316	-1.180870	-0.061037
1	-1.297048	2.046190	0.112501	1	-1.468325	1.995722	0.105553	1	-1.457305	2.000400	0.098480
	M34 CBS-QB3				M34 CBS-APNO				M34 G3		
6	-0.066209	-1.217053	0.134804	6	-0.061520	-1.208993	0.160699	6	-0.063144	-1.211255	0.151034
6	0.893485	-0.029088	0.009955	6	0.887838	-0.027660	0.011171	6	0.886833	-0.028223	0.009827
6	0.078374	1.272755	0.038611	6	0.086057	1.269970	0.033708	6	0.089086	1.272068	0.034238
6	-1.342590	0.828273	0.039800	6	-1.342920	0.820737	0.087454	6	-1.341208	0.825222	0.079961
6	-1.478641	-0.658274	-0.127674	6	-1.460704	-0.662462	-0.161082	6	-1.466999	-0.661074	-0.150126
1	-1.809732	-0.912015	-1.147420	1	-1.715268	-0.857229	-1.204115	1	-1.746320	-0.869855	-1.183109
1	-2.187654	1.503827	0.048989	1	-2.177872	1.494207	0.025967	1	-2.173830	1.500322	0.011752
1	0.368448	1.862389	0.920871	1	0.390169	1.871049	0.887908	1	0.389856	1.867676	0.893627
1	0.361896	1.891797	-0.826452	1	0.327997	1.850377	-0.856097	1	0.336600	1.859457	-0.848899
8	2.090444	-0.102562	-0.091731	8	2.062651	-0.102111	-0.102754	8	2.067564	-0.105160	-0.098256
1	0.242707	-2.021691	-0.534191	1	0.259820	-2.035388	-0.460122	1	0.250412	-2.026255	-0.488731
1	-2.233925	-1.085749	0.540994	1	-2.238333	-1.122623	0.439513	1	-2.232666	-1.111235	0.473141
1	0.028192	-1.597743	1.158081	1	-0.000221	-1.533056	1.197275	1	0.008026	-1.559261	1.178668
	M35 CBS-QB3				M35 CBS-APNO				M35 G3		
6	-0.806868	0.947842	0.132370	6	-0.805240	0.947872	0.131785	6	-0.804968	0.955416	0.126254
6	-1.481918	-0.322617	-0.372100	6	-1.477421	-0.327053	-0.355346	6	-1.461634	-0.329111	-0.357092
6	2.220197	-0.949061	-0.161707	6	2.208194	-0.943518	-0.161971	6	2.189066	-0.953117	-0.163535

Table 13: Cartesian coordinates for minima (M28–M35) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	1.525355	0.009183	0.442963	6	1.520059	0.004957	0.440187	6	1.513739	0.003418	0.442446
6	0.677892	1.035806	-0.257039	6	0.673074	1.034706	-0.258273	6	0.677072	1.044111	-0.253155
1	0.774365	0.924839	-1.340711	1	0.771130	0.928252	-1.333620	1	0.781597	0.945938	-1.328495
1	1.545659	0.073151	1.530264	1	1.543641	0.066051	1.518552	1	1.537167	0.062093	1.520132
1	2.809765	-1.664247	0.400496	1	2.793372	-1.652779	0.396539	1	2.764914	-1.673285	0.389582
1	2.223915	-1.053734	-1.242351	1	2.213127	-1.047489	-1.234307	1	2.193997	-1.054587	-1.235413
8	-2.359293	-0.928922	0.132412	8	-2.344201	-0.924797	0.124441	8	-2.334691	-0.929328	0.126435
1	-1.367031	1.769439	-0.330052	1	-1.362990	1.759820	-0.328190	1	-1.360973	1.764637	-0.340078
1	1.034519	2.040426	-0.001245	1	1.031410	2.028207	0.000145	1	1.035442	2.035000	0.013802
1	-0.954799	1.014584	1.217377	1	-0.948069	1.014541	1.207063	1	-0.954272	1.030527	1.199484

Table 14: Cartesian coordinates for minima (M36–M40) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M36 CBS-QB3				M36 CBS-APNO				M36 G3		
6	-0.674190	0.117638	0.003781	6	-0.661212	0.113469	0.002717	6	-0.661849	0.114872	0.003086
6	0.177664	1.145552	0.000080	6	0.169525	1.137434	-0.000360	6	0.172092	1.137719	0.001910
6	1.332021	-0.854292	-0.082199	6	1.322926	-0.857526	-0.100037	6	1.323733	-0.859719	-0.100359
8	-0.025138	-1.108014	0.008102	8	-0.025574	-1.094102	0.009540	8	-0.026640	-1.095452	0.007370
1	-0.099533	2.188542	-0.001379	1	-0.117661	2.169351	-0.001578	1	-0.109619	2.171314	0.000875
6	-2.158603	0.039766	0.002063	6	-2.146992	0.038057	0.003194	6	-2.149068	0.039495	0.003385
1	-2.515830	-0.489842	-0.886231	1	-2.493032	-0.496575	-0.875888	1	-2.498611	-0.491999	-0.875714
1	-2.516441	-0.511172	0.877044	1	-2.491987	-0.504189	0.878083	1	-2.497612	-0.503230	0.876082
1	-2.594071	1.039271	0.014196	1	-2.579338	1.030509	0.008169	1	-2.582102	1.031433	0.010465
6	1.593536	0.618848	0.009554	6	1.588618	0.621824	0.012408	6	1.590257	0.620766	0.010732
1	2.197935	0.997821	-0.828802	1	2.188125	0.992912	-0.816685	1	2.187143	0.991904	-0.820244
1	2.143126	0.904692	0.924052	1	2.120295	0.882329	0.929222	1	2.127080	0.882928	0.923485
1	1.963354	-1.670275	0.236615	1	1.940998	-1.641071	0.294820	1	1.935846	-1.637533	0.313569
	M37 CBS-QB3				M37 CBS-APNO				M37 G3		
6	-1.851375	-0.284318	-0.000049	6	-1.877695	-0.248837	0.000032	6	-1.875921	-0.252480	0.000024
6	-1.113567	1.033585	0.000178	6	-1.085801	1.034409	0.000218	6	-1.091470	1.036277	0.000220
6	0.391969	0.990251	-0.000182	6	0.417738	0.954465	-0.000191	6	0.412517	0.957931	-0.000193
6	1.154809	-0.074979	0.000222	6	1.167578	-0.133334	0.000292	6	1.163132	-0.133921	0.000299
8	-1.355972	-1.379591	-0.000168	8	-1.446825	-1.347338	-0.000379	8	-1.433120	-1.352699	-0.000385
1	-1.487795	1.601942	-0.865497	1	-1.430963	1.606365	-0.862450	1	-1.437357	1.609079	-0.861365
1	0.870035	1.979411	-0.000820	1	0.915957	1.918794	-0.000860	1	0.907128	1.923023	-0.000870
6	2.584507	-0.409989	0.000030	6	2.624049	-0.409937	0.000081	6	2.621921	-0.405414	0.000087
1	2.852178	-1.002427	-0.880663	1	2.906976	-0.984828	-0.876265	1	2.909386	-0.979486	-0.875096
1	3.209792	0.497135	-0.000714	1	3.195366	0.517748	-0.000664	1	3.193389	0.521640	-0.000663
1	2.852680	-1.001330	0.881306	1	2.907449	-0.983709	0.877009	1	2.909857	-0.978358	0.875855
1	-2.959762	-0.166682	0.000131	1	-2.964848	-0.082133	0.000279	1	-2.961583	-0.097234	0.000287
1	-1.487408	1.601376	0.866404	1	-1.430548	1.605862	0.863393	1	-1.436940	1.608567	0.862319
	M38 CBS-QB3				M38 CBS-APNO				M38 G3		
6	-2.436648	-0.805208	0.037308	6	-2.412585	-0.827684	0.026778	6	-2.395357	-0.839975	0.031190
6	-1.695077	0.399879	-0.352641	6	-1.717653	0.427166	-0.349523	6	-1.718911	0.424692	-0.350147
6	-0.550375	1.014421	-0.183331	6	-0.555637	1.026772	-0.151415	6	-0.559516	1.037665	-0.152663
6	0.603978	0.497337	0.670152	6	0.593678	0.465208	0.663502	6	0.597552	0.488076	0.660446
6	1.790050	0.111679	-0.192606	6	1.772927	0.105959	-0.211182	6	1.762818	0.101162	-0.221603

Table 14: Cartesian coordinates for minima (M36–M40) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
8	2.328454	-0.964394	-0.167779	8	2.346661	-0.925979	-0.162544	8	2.335577	-0.936838	-0.151953
1	-1.848635	-1.442195	0.715306	1	-1.779153	-1.466324	0.638599	1	-1.756695	-1.467521	0.648338
1	-2.696183	-1.407507	-0.838876	1	-2.695802	-1.385966	-0.859849	1	-2.668361	-1.409196	-0.851516
1	-3.370622	-0.547795	0.546743	1	-3.317370	-0.610516	0.585892	1	-3.305732	-0.637201	0.586308
1	-0.374899	1.965772	-0.686607	1	-0.393417	1.992359	-0.607585	1	-0.405136	2.003373	-0.609599
1	0.319393	-0.368805	1.268694	1	0.309957	-0.413824	1.226299	1	0.315440	-0.377094	1.245159
1	0.930404	1.297534	1.348652	1	0.933369	1.223237	1.368958	1	0.948595	1.256751	1.348284
1	2.141336	0.909492	-0.884970	1	2.084749	0.884338	-0.920924	1	2.067749	0.855866	-0.954696
	M39 CBS-QB3				M39 CBS-APNO				M39 G3		
6	2.739535	-0.586586	0.041984	6	2.751824	-0.562355	0.037817	6	2.755384	-0.561842	0.038390
6	1.333094	-0.166808	0.027147	6	1.312790	-0.207215	0.020854	6	1.314171	-0.210130	0.028106
6	0.600278	0.919543	0.016667	6	0.592829	0.901117	0.019916	6	0.594659	0.903142	0.014046
6	-0.910936	0.968471	0.016185	6	-0.916302	0.966576	0.023152	6	-0.915032	0.965576	0.026094
6	-1.557800	-0.359972	-0.319892	6	-1.582543	-0.338437	-0.339724	6	-1.578096	-0.341653	-0.337254
8	-2.504771	-0.820682	0.262365	8	-2.461652	-0.828663	0.279758	8	-2.475350	-0.823497	0.273729
1	2.986419	-1.191984	-0.835662	1	3.020200	-1.141350	-0.840167	1	3.019893	-1.154790	-0.831247
1	2.966317	-1.185969	0.929137	1	2.992775	-1.154935	0.914577	1	3.007775	-1.140248	0.921184
1	3.409080	0.287565	0.046705	1	3.365641	0.336976	0.054403	1	3.370480	0.336153	0.035173
1	1.104744	1.894294	0.017286	1	1.108996	1.854255	0.039834	1	1.108440	1.856743	0.014382
1	-1.247356	1.690602	-0.742650	1	-1.241026	1.703648	-0.711566	1	-1.246636	1.706735	-0.700954
1	-1.307185	1.314058	0.975915	1	-1.294067	1.286363	0.988643	1	-1.290408	1.280300	0.994113
1	-1.098875	-0.890994	-1.182200	1	-1.210894	-0.813773	-1.255873	1	-1.193257	-0.827473	-1.238775
	M40 CBS-QB3				M40 CBS-APNO				M40 G3		
6	2.735241	-0.482842	-0.026171	6	2.731941	-0.480271	-0.024383	6	2.732399	-0.482288	-0.027264
6	1.489523	0.319282	-0.257759	6	1.482683	0.320686	-0.254311	6	1.485506	0.325379	-0.249836
6	0.342894	0.162382	0.401021	6	0.343503	0.149026	0.388879	6	0.341317	0.144535	0.387059
6	-0.896102	0.968887	0.141707	6	-0.893856	0.964973	0.140293	6	-0.893909	0.965673	0.146390
6	-2.120489	0.127997	-0.249899	6	-2.109804	0.121816	-0.233642	6	-2.105114	0.124716	-0.252776
8	-2.293257	-1.027198	-0.084159	8	-2.295344	-1.010962	-0.088567	8	-2.300459	-1.010480	-0.082291
1	3.571245	0.162435	0.265435	1	3.552072	0.164608	0.281018	1	3.554003	0.153091	0.292625
1	3.043115	-1.001387	-0.940892	1	3.039871	-0.981053	-0.938661	1	3.045345	-0.970515	-0.946250
1	2.592052	-1.230550	0.756965	1	2.585116	-1.232229	0.742723	1	2.581280	-1.246220	0.726787
1	0.257600	-0.609880	1.161850	1	0.257482	-0.623377	1.136027	1	0.249664	-0.638889	1.120778
1	-0.744127	1.724574	-0.632363	1	-0.743746	1.704196	-0.637085	1	-0.736188	1.721274	-0.613453

Table 14: Cartesian coordinates for minima (M36–M40) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-1.229945	1.510877	1.037486	1	-1.201276	1.507137	1.033043	1	-1.206973	1.489866	1.047841
1	1.549709	1.087288	-1.028605	1	1.546433	1.091034	-1.009539	1	1.555347	1.107143	-0.991431

Table 15: Cartesian coordinates for minima (M41–M48) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	M41 CBS-QB3				M41 CBS-APNO				M41 G3		
6	0.682677	0.094983	-0.000004	6	0.676720	0.096931	0.000006	6	0.677601	0.098476	0.000006
6	-0.157072	1.196196	-0.000002	6	-0.152641	1.199821	0.000004	6	-0.154179	1.201415	0.000004
6	-1.443116	-0.737802	-0.000002	6	-1.426902	-0.747369	0.000008	6	-1.427776	-0.748090	0.000005
8	-0.032333	-1.074574	0.000001	8	-0.042489	-1.059379	-0.000010	8	-0.042866	-1.060203	-0.000006
1	0.181820	2.222117	0.000002	1	0.183458	2.217766	0.000013	1	0.179336	2.220354	0.000010
6	2.158931	-0.037727	0.000002	6	2.155438	-0.045409	-0.000001	6	2.157492	-0.045680	-0.000001
1	2.506001	-0.590661	0.880906	1	2.487717	-0.595344	0.876792	1	2.492337	-0.594827	0.875725
1	2.506007	-0.590668	-0.880896	1	2.487712	-0.595306	-0.876819	1	2.492332	-0.594792	-0.875752
1	2.631507	0.945507	-0.000001	1	2.630842	0.928454	0.000019	1	2.634505	0.927132	0.000017
6	-1.473235	0.759822	0.000003	6	-1.470826	0.755616	-0.000012	6	-1.472005	0.755427	-0.000010
1	-2.371871	1.356745	0.000001	1	-2.366522	1.343388	-0.000017	1	-2.368649	1.341804	-0.000011
1	-1.901949	-1.199642	-0.886217	1	-1.887021	-1.190743	-0.879893	1	-1.886862	-1.193679	-0.878411
1	-1.901958	-1.199637	0.886219	1	-1.887007	-1.190718	0.879941	1	-1.886858	-1.193661	0.878441
	M42 CBS-QB3				M42 CBS-APNO				M42 G3		
6	-0.835461	0.154691	-0.000010	6	-0.845085	0.158474	-0.000010	6	-0.844527	0.154909	-0.000010
6	0.184554	-0.899372	0.000015	6	0.180830	-0.891299	0.000026	6	0.179502	-0.892572	0.000028
6	1.575997	-0.718007	0.000020	6	1.575605	-0.714140	0.000028	6	1.575472	-0.715355	0.000030
6	2.256108	0.475178	0.000000	6	2.278439	0.475921	-0.000005	6	2.280121	0.474928	-0.000006
8	-0.566073	1.349376	-0.000034	8	-0.579148	1.331216	-0.000047	8	-0.576704	1.334212	-0.000049
1	-0.182495	-1.921333	0.000033	1	-0.182188	-1.905160	0.000056	1	-0.183299	-1.906231	0.000060
1	2.168372	-1.630571	0.000041	1	2.153631	-1.624512	0.000060	1	2.152877	-1.625491	0.000063
6	-2.282194	-0.316758	0.000004	6	-2.284276	-0.312432	0.000004	6	-2.286311	-0.310780	0.000004
1	-2.942601	0.549012	-0.000131	1	-2.943312	0.544573	-0.000092	1	-2.942431	0.548355	-0.000085
1	-2.487837	-0.933238	-0.880936	1	-2.482875	-0.922869	-0.876539	1	-2.491778	-0.919814	-0.875545
1	-2.487882	-0.932982	0.881115	1	-2.482904	-0.922689	0.876667	1	-2.491804	-0.919647	0.875665
1	3.339657	0.482559	0.000006	1	3.353474	0.456128	0.000001	1	3.354601	0.456396	0.000000
1	1.727345	1.417157	-0.000022	1	1.784272	1.425659	-0.000038	1	1.789925	1.425953	-0.000040
	M43 CBS-QB3				M43 CBS-APNO				M43 G3		
6	-1.000869	-0.101949	0.000020	6	-0.999225	-0.103169	-0.000583	6	0.995645	-0.102475	-0.000049
6	0.182929	-0.967796	-0.000018	6	0.181956	-0.967049	-0.000186	6	-0.180229	-0.968720	0.000111
6	1.556548	-0.673600	-0.000034	6	1.558812	-0.669461	0.000036	6	-1.558423	-0.671712	0.000128
6	2.205609	0.536259	-0.000081	6	2.211079	0.548616	-0.000016	6	-2.211144	0.547361	-0.000039
8	-2.105816	-0.633739	-0.000097	8	-2.083125	-0.641932	0.000363	8	2.087428	-0.640719	-0.000136

Table 15: Cartesian coordinates for minima (M41–M48) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-0.095409	-2.016724	-0.000052	1	-0.086387	-2.008778	-0.000023	1	0.088571	-2.009765	0.000191
1	2.198396	-1.552086	-0.000020	1	2.195354	-1.539524	0.000292	1	-2.194969	-1.541059	0.000250
6	-0.886349	1.411324	0.000183	6	-0.911257	1.405682	0.000099	6	0.907941	1.406937	0.000000
1	-1.891679	1.830039	0.000377	1	-1.916188	1.804394	0.000709	1	1.912522	1.806309	-0.000406
1	-0.347113	1.764859	0.883750	1	-0.384332	1.762772	0.879002	1	0.382557	1.768175	-0.877788
1	-0.347407	1.765041	-0.883494	1	-0.385110	1.763526	-0.878955	1	0.383284	1.768195	0.878207
1	3.288158	0.565765	-0.000089	1	3.285546	0.571278	0.000198	1	-3.284987	0.572599	-0.000030
1	1.694375	1.487586	-0.000117	1	1.707930	1.494068	-0.000224	1	-1.709141	1.492953	-0.000244
	M44 CBS-QB3				M44 CBS-APNO				M44 G3		
6	1.037867	-0.038514	-0.017438	6	1.031429	-0.024184	-0.015920	6	1.029232	-0.020861	-0.015696
6	-0.114786	-0.944901	-0.288167	6	-0.100002	-0.952544	-0.208144	6	-0.094867	-0.956742	-0.190999
6	-1.424944	-0.707031	-0.151801	6	-1.422247	-0.728968	-0.120096	6	-1.422720	-0.737376	-0.111312
6	-2.118094	0.540017	0.312960	6	-2.151734	0.537597	0.238945	6	-2.156264	0.535115	0.221425
8	2.102002	-0.525392	0.394149	8	2.130696	-0.519392	0.295982	8	2.144087	-0.513858	0.272259
1	0.205395	-1.946846	-0.558106	1	0.227332	-1.958579	-0.407746	1	0.237188	-1.964360	-0.370978
1	-2.092581	-1.537238	-0.374040	1	-2.057060	-1.579464	-0.310251	1	-2.053601	-1.592708	-0.287285
6	0.966358	1.368964	-0.298311	6	0.961795	1.382464	-0.225024	6	0.950930	1.386896	-0.207666
1	1.830222	1.974467	-0.053170	1	1.846536	1.961213	-0.036486	1	1.835136	1.968671	-0.030718
1	0.129828	1.822973	-0.812808	1	0.093138	1.869672	-0.620670	1	0.075046	1.877064	-0.581387
1	-1.439785	1.272840	0.749575	1	-1.551720	1.210356	0.837525	1	-1.578206	1.194315	0.856007
1	-2.871073	0.286940	1.065815	1	-3.045116	0.295442	0.804922	1	-3.079653	0.302256	0.740265
1	-2.656416	1.018779	-0.513925	1	-2.474130	1.070303	-0.653725	1	-2.426472	1.083437	-0.678493
	M45 CBS-QB3				M45 CBS-APNO				M45 G3		
6	-0.958206	-0.122294	0.000001	6	-0.972100	-0.106348	-0.000017	6	-0.973307	-0.102042	0.000089
6	0.078605	0.943533	0.000107	6	0.075689	0.932149	0.000090	6	0.073314	0.933827	0.000119
6	1.410558	0.781162	0.000058	6	1.410595	0.772834	0.000067	6	1.411909	0.774186	0.000054
6	2.197586	-0.490923	-0.000093	6	2.224832	-0.488546	-0.000073	6	2.226456	-0.488071	-0.000075
8	-0.704861	-1.337534	0.000055	8	-0.712674	-1.319383	0.000027	8	-0.710419	-1.321584	-0.000039
1	-0.304498	1.960063	0.000210	1	-0.294931	1.943927	0.000188	1	-0.296603	1.945559	0.000206
1	2.006970	1.692565	0.000141	1	1.990358	1.683303	0.000168	1	1.992366	1.683312	0.000125
6	-2.331347	0.311918	-0.000107	6	-2.342681	0.297081	-0.000084	6	-2.344599	0.294293	-0.000087
1	-3.105647	-0.444518	-0.000178	1	-3.100501	-0.463260	-0.000110	1	-3.100786	-0.466826	-0.000217
1	-2.612110	1.358375	-0.000114	1	-2.634838	1.330948	-0.000105	1	-2.643289	1.325687	-0.000116
1	1.558737	-1.368756	-0.000476	1	1.617291	-1.377665	-0.000493	1	1.618909	-1.377245	-0.000428

Table 15: Cartesian coordinates for minima (M41–M48) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.855885	-0.519163	0.876331	1	2.872745	-0.502861	0.873650	1	2.874855	-0.505711	0.872748
1	2.856380	-0.518669	-0.876154	1	2.873254	-0.502340	-0.873422	1	2.875261	-0.505264	-0.872602
	M46 CBS-QB3				M46 CBS-APNO				M46 G3		
6	-1.131262	0.171783	-0.098688	6	-1.117784	0.187228	-0.071427	6	-1.120799	0.182333	-0.067976
6	-0.040747	-0.753090	-0.570319	6	-0.060492	-0.710739	-0.572832	6	-0.059320	-0.707249	-0.576486
6	1.358160	-0.348768	-0.550414	6	1.375998	-0.355670	-0.549953	6	1.375937	-0.340495	-0.561916
6	1.923362	0.599783	0.453961	6	1.952631	0.610083	0.442437	6	1.956164	0.606755	0.447026
8	-1.615811	1.258691	-0.208057	8	-1.684862	1.207086	-0.192966	8	-1.702534	1.202134	-0.184633
1	-0.323718	-1.436103	-1.366410	1	-0.360507	-1.336711	-1.397830	1	-0.356805	-1.331633	-1.404289
1	1.943505	-0.571655	-1.435217	1	1.938506	-0.573452	-1.440540	1	1.926223	-0.522466	-1.467552
6	-0.919046	-0.995631	0.747916	6	-0.888687	-1.004659	0.735852	6	-0.874434	-1.010586	0.733040
1	-1.591189	-1.842921	0.667184	1	-1.587755	-1.821542	0.681211	1	-1.568722	-1.832604	0.685510
1	-0.477618	-0.851627	1.730417	1	-0.402448	-0.882716	1.689127	1	-0.383129	-0.890489	1.684248
1	1.646224	1.643722	0.237110	1	1.620774	1.630378	0.247152	1	1.601340	1.625863	0.293860
1	3.014551	0.553711	0.466180	1	3.035719	0.601777	0.397909	1	3.037676	0.622635	0.378270
1	1.571936	0.390882	1.470449	1	1.664620	0.368121	1.462237	1	1.698400	0.327072	1.464882
	M47 CBS-QB3				M47 CBS-APNO				M47 G3		
6	1.883223	0.233325	-0.191661	6	1.863218	0.203823	-0.211570	6	1.858485	0.202742	-0.224133
6	-0.531003	0.949159	-0.031647	6	-0.532452	0.944063	-0.031181	6	-0.535708	0.944850	-0.027651
6	-1.744541	0.463733	-0.296005	6	-1.734625	0.464231	-0.291156	6	-1.739203	0.465234	-0.287174
6	-2.287274	-0.901890	0.009219	6	-2.286684	-0.901398	0.008502	6	-2.288995	-0.903169	0.005914
8	2.665374	-0.641852	-0.305596	8	2.665489	-0.625366	-0.295296	8	2.677687	-0.622254	-0.287055
1	-0.305712	1.968329	-0.333501	1	-0.316362	1.957227	-0.329403	1	-0.320859	1.959428	-0.320105
1	-2.442997	1.133939	-0.792623	1	-2.426199	1.130736	-0.783026	1	-2.433680	1.131982	-0.773009
6	0.600628	0.231259	0.649087	6	0.606035	0.234680	0.650724	6	0.606812	0.234015	0.646713
1	0.880078	0.762290	1.569745	1	0.894579	0.780348	1.547604	1	0.899435	0.774969	1.545155
1	0.368085	-0.802885	0.917755	1	0.375513	-0.782503	0.939988	1	0.374802	-0.782141	0.938014
1	-2.641727	-1.386636	-0.906669	1	-2.627502	-1.374607	-0.908465	1	-2.634730	-1.372573	-0.910825
1	-3.151106	-0.831509	0.679551	1	-3.148758	-0.820574	0.665675	1	-3.147240	-0.830881	0.668582
1	-1.555806	-1.562230	0.476552	1	-1.568133	-1.560081	0.478088	1	-1.567566	-1.564788	0.466606
	M48 CBS-QB3				M48 CBS-APNO				M48 G3		
6	1.888253	-0.542927	-0.169915	6	1.896682	-0.524650	-0.165058	6	1.885531	-0.533491	-0.185100
6	-0.281207	0.591479	0.524530	6	-0.278095	0.581097	0.495227	6	-0.275293	0.582663	0.492878
6	-1.532673	0.676227	0.069160	6	-1.528074	0.674388	0.075785	6	-1.527304	0.676745	0.071708

Table 15: Cartesian coordinates for minima (M41–M48) on the C_5H_7O potential energy surface.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	-2.410138	-0.425030	-0.450186	6	-2.433786	-0.412833	-0.431643	6	-2.436203	-0.411929	-0.428153
8	2.427863	0.427285	-0.568162	8	2.444794	0.425208	-0.533186	8	2.451870	0.425900	-0.523235
1	0.212209	1.502940	0.848988	1	0.218838	1.481251	0.815397	1	0.225337	1.482282	0.806563
1	-1.990634	1.663311	0.071934	1	-1.973426	1.657134	0.095478	1	-1.971057	1.659505	0.083734
6	0.566756	-0.645418	0.607508	6	0.565964	-0.661949	0.569657	6	0.566093	-0.661212	0.574774
1	0.888849	-0.843930	1.639174	1	0.844897	-0.882250	1.598941	1	0.860554	-0.864732	1.603134
1	0.057278	-1.550151	0.274824	1	0.069835	-1.544275	0.191472	1	0.058860	-1.547236	0.221064
1	-2.730627	-0.208555	-1.475024	1	-2.770015	-0.179188	-1.438386	1	-2.774911	-0.186110	-1.435543
1	-3.322366	-0.506610	0.151043	1	-3.320838	-0.483148	0.192711	1	-3.322815	-0.480230	0.196560
1	-1.923565	-1.401267	-0.452226	1	-1.963789	-1.387504	-0.453939	1	-1.967879	-1.387327	-0.446266

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
	TS1 CBS-QB3				TS1 CBS-APNO				TS1 G3		
6	1.429601	-0.054846	0.338495	6	1.403890	-0.134241	0.329556	6	1.406305	-0.134398	0.329264
6	0.813886	1.110723	0.062061	6	0.876361	1.069055	0.101008	6	0.878424	1.069266	0.099985
6	-0.429571	0.710126	-0.577947	6	-0.381303	0.763224	-0.559233	6	-0.379441	0.762793	-0.557690
6	-0.473886	-0.707602	-0.722768	6	-0.508112	-0.619272	-0.740908	6	-0.511338	-0.620666	-0.741610
8	0.695095	-1.130812	-0.057898	8	0.627975	-1.125951	-0.094557	8	0.625986	-1.127747	-0.092677
1	2.382744	-0.273077	0.798026	1	2.331756	-0.413958	0.787681	1	2.333796	-0.417737	0.784642
1	1.169086	2.105513	0.277494	1	1.284474	2.024142	0.354634	1	1.284958	2.026096	0.350854
1	-1.081858	1.371024	-1.131743	1	-1.024884	1.473662	-1.038252	1	-1.020731	1.476547	-1.035301
6	-1.706733	-0.048632	0.577458	6	-1.694785	-0.053506	0.572424	6	-1.694038	-0.050969	0.570636
1	-2.644092	-0.203810	0.057615	1	-2.640622	-0.071307	0.060708	1	-2.640530	-0.055669	0.059634
1	-1.461656	-0.881093	1.228124	1	-1.530269	-0.954361	1.138236	1	-1.544341	-0.955890	1.133956
1	-1.724772	0.869321	1.169864	1	-1.620568	0.797860	1.236364	1	-1.620510	0.792474	1.244124
	TS2 CBS-QB3				TS2 CBS-APNO				TS2 G3		
6	-1.550163	0.538402	-0.033105	6	-1.538129	0.530778	-0.041553	6	-1.535988	0.531454	-0.041602
6	-0.233650	1.150716	-0.007636	6	-0.227378	1.143250	-0.006470	6	-0.228026	1.144454	-0.005424
6	0.630355	0.112927	-0.004364	6	0.614398	0.102109	-0.004989	6	0.615308	0.102839	-0.004345
8	-0.051041	-1.079237	0.001881	8	-0.045898	-1.057120	-0.003105	8	-0.046874	-1.057470	-0.001444
1	0.010548	2.200381	0.007977	1	0.019462	2.183035	0.017393	1	0.015517	2.185357	0.019257
6	2.113699	0.024717	0.006216	6	2.100188	0.021407	0.008825	6	2.102544	0.019908	0.007927
1	2.462069	-0.498289	0.901282	1	2.434613	-0.512150	0.892260	1	2.440342	-0.514002	0.889418
1	2.465288	-0.541445	-0.860796	1	2.444628	-0.526892	-0.861575	1	2.448468	-0.526912	-0.862349
1	2.560918	1.018696	-0.016896	1	2.538242	1.010989	0.002900	1	2.543020	1.008158	0.002554
6	-1.424272	-0.896531	-0.100200	6	-1.415284	-0.871969	-0.101947	6	-1.420392	-0.871248	-0.104120
1	-1.812685	-0.168679	0.990692	1	-1.788563	-0.280507	0.988312	1	-1.793527	-0.292198	0.982892
1	-2.493623	1.041842	-0.202774	1	-2.483970	1.029033	-0.137649	1	-2.479503	1.034912	-0.134832
	TS3 CBS-QB3				TS3 CBS-APNO				TS3 G3		
6	0.003612	-1.208487	0.190299	6	-0.029777	-1.212805	0.189446	6	-0.017078	-1.215087	0.191421
6	0.776789	-0.077130	0.480871	6	0.775428	-0.091511	0.486958	6	0.785342	-0.097147	0.490966
6	-0.527003	1.305328	0.172858	6	-0.504422	1.299413	0.169113	6	-0.522640	1.310010	0.169660
6	-1.659493	0.958111	-0.197381	6	-1.600687	0.886117	-0.197050	6	-1.609956	0.871450	-0.196873
8	-1.109278	-1.369108	-0.157790	8	-1.142246	-1.240131	-0.158460	8	-1.138187	-1.238439	-0.159602
1	0.971533	-0.004510	1.554147	1	0.964149	-0.015746	1.550338	1	0.977380	-0.013654	1.552050
1	0.056902	2.180616	0.405102	1	0.038428	2.190326	0.390528	1	0.018001	2.201512	0.391856

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	2.002699	0.199231	-0.379803	6	1.997322	0.161106	-0.378849	6	1.998686	0.169955	-0.381645
1	2.836091	-0.459456	-0.127379	1	2.800768	-0.523599	-0.133916	1	2.811610	-0.507260	-0.146785
1	1.769681	0.079830	-1.439529	1	1.754057	0.053079	-1.429524	1	1.750598	0.065225	-1.430933
1	2.330063	1.228427	-0.215308	1	2.356159	1.170220	-0.209918	1	2.350500	1.180870	-0.212167
1	-2.669668	0.865645	-0.515776	1	-2.602776	0.792857	-0.517541	1	-2.608715	0.745725	-0.518378
	TS4 CBS-QB3				TS4 CBS-APNO				TS4 G3		
6	-1.010330	0.497589	0.000007	6	-0.916639	0.499158	0.000057	6	-0.918022	0.509926	0.000026
6	-0.070701	1.309402	0.000042	6	0.008347	1.306534	-0.000007	6	0.010325	1.315457	0.000048
6	1.492491	-0.779080	-0.000037	6	1.413041	-0.862553	-0.000087	6	1.410494	-0.868443	-0.000044
8	0.510125	-1.429671	-0.000062	8	0.347999	-1.338688	-0.000017	8	0.333765	-1.337088	-0.000051
1	0.141906	2.363938	0.000077	1	0.227710	2.349588	-0.000026	1	0.243623	2.355605	0.000085
6	-2.279362	-0.219153	0.000020	6	-2.225717	-0.163480	0.000144	6	-2.223617	-0.162841	0.000012
1	-2.364185	-0.863291	-0.879824	1	-2.328138	-0.791708	-0.876695	1	-2.324571	-0.792505	-0.875694
1	-2.364144	-0.863326	0.879843	1	-2.328018	-0.791713	0.876994	1	-2.324573	-0.792536	0.875695
1	-3.135109	0.468245	0.000054	1	-3.025517	0.571961	0.000201	1	-3.031336	0.563393	0.000024
6	1.734721	0.593222	0.000016	6	1.752361	0.502075	-0.000115	6	1.764234	0.489657	0.000003
1	2.219808	0.959994	-0.904742	1	2.240750	0.840485	-0.902227	1	2.253117	0.830134	-0.899955
1	2.219805	0.959924	0.904804	1	2.240865	0.840494	0.901932	1	2.253134	0.830069	0.899975
	TS5 CBS-QB3				TS5 CBS-APNO				TS5 G3		
6	0.224799	1.282731	-0.050411	6	0.209595	1.266222	-0.065200	6	0.208200	1.266103	-0.066025
6	1.537924	0.641910	-0.061293	6	1.541853	0.622354	-0.046633	6	1.541138	0.622510	-0.046024
6	1.386266	-0.703989	-0.045247	6	1.380484	-0.697299	-0.028918	6	1.383280	-0.697769	-0.027929
8	0.087471	-1.071419	0.062145	8	0.078949	-1.039446	0.045367	8	0.077786	-1.040711	0.046468
1	2.483704	1.161148	-0.113125	1	2.479307	1.137656	-0.088811	1	2.477701	1.140007	-0.085958
6	-0.623311	0.149077	0.096896	6	-0.610144	0.134911	0.051556	6	-0.608154	0.134714	0.047205
1	-0.398641	0.822643	1.115243	1	-0.359137	0.875601	1.071638	1	-0.359899	0.901600	1.060397
6	-2.102427	-0.000948	-0.098158	6	-2.095747	-0.003957	-0.071279	6	-2.095564	-0.005244	-0.069356
1	-2.521546	-0.756142	0.569598	1	-2.483503	-0.715734	0.648200	1	-2.484008	-0.707837	0.657952
1	-2.589018	0.957630	0.078378	1	-2.562753	0.960445	0.072195	1	-2.562724	0.960191	0.064259
1	-2.304169	-0.303203	-1.128571	1	-2.333390	-0.360983	-1.067474	1	-2.337736	-0.372770	-1.060132
1	2.090405	-1.523414	-0.069404	1	2.071633	-1.514809	-0.035838	1	2.070971	-1.517392	-0.035493
					TS6 CBS-APNO				TS6 G3		
				6	0.768439	0.240417	0.490019	6	0.767112	0.242469	0.493139
				6	-0.111898	1.285751	0.176239	6	-0.111597	1.288855	0.179247

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
				6	-1.331297	0.814664	-0.195576	6	-1.329643	0.813777	-0.196900
				6	-1.357121	-0.614727	-0.151002	6	-1.356473	-0.612960	-0.152758
				8	-0.336828	-1.210419	0.187435	8	-0.333949	-1.214976	0.190516
				1	0.903767	0.051380	1.543734	1	0.908282	0.050483	1.544230
				1	-2.189448	1.392379	-0.481790	1	-2.188395	1.389629	-0.486062
				6	1.946973	-0.080372	-0.384389	6	1.942638	-0.079613	-0.387133
				1	2.728369	0.643044	-0.176010	1	2.723655	0.647849	-0.194616
				1	2.319291	-1.072899	-0.169428	1	2.322735	-1.067735	-0.168175
				1	1.679051	-0.006539	-1.430727	1	1.665884	-0.018196	-1.431510
				1	-2.236976	-1.198413	-0.397000	1	-2.232786	-1.197382	-0.401572
	TS7 CBS-QB3				TS7 CBS-APNO				TS7 G3		
6	-1.616736	-0.151596	-0.561445	6	-1.606142	-0.106481	-0.571864	6	-1.608163	-0.112786	-0.572492
6	-0.441277	0.350180	-0.300200	6	-0.437320	0.360969	-0.272004	6	-0.437748	0.359340	-0.278163
6	0.742137	0.825366	-0.030768	6	0.737610	0.815739	0.026409	6	0.738175	0.816351	0.020536
6	1.873189	-0.039774	0.478111	6	1.865312	-0.077286	0.468210	6	1.864248	-0.072270	0.471262
8	2.658304	-0.605170	-0.233786	8	2.638618	-0.575383	-0.270420	8	2.643476	-0.577890	-0.266060
1	-1.794890	-0.529994	-1.566992	1	-1.779019	-0.396944	-1.596452	1	-1.785572	-0.415290	-1.592213
1	0.972196	1.882122	-0.163168	1	0.950887	1.871995	-0.028555	1	0.952689	1.871617	-0.044103
6	-2.759200	-0.246348	0.418260	6	-2.744590	-0.273510	0.401464	6	-2.745837	-0.269563	0.404320
1	-3.631610	0.300935	0.047061	1	-3.604390	0.306863	0.079569	1	-3.606877	0.307346	0.080826
1	-3.065408	-1.288670	0.553069	1	-3.050615	-1.314533	0.449422	1	-3.054340	-1.308813	0.464814
1	-2.484718	0.161491	1.391821	1	-2.462715	0.049990	1.395680	1	-2.463174	0.062965	1.395176
1	1.949312	-0.111490	1.584753	1	1.947686	-0.230892	1.550404	1	1.945421	-0.221136	1.551207
	TS8 CBS-QB3				TS8 CBS-APNO						
6	1.215642	0.010170	0.522557	6	1.112947	0.039487	0.508824				
6	0.511072	1.143286	0.054854	6	0.527538	1.247043	0.038497				
6	-0.747739	1.134079	-0.220360	6	-0.769434	1.123234	-0.215288				
6	-1.348676	-0.386557	0.075545	6	-1.278655	-0.250436	0.035144				
8	-2.423761	-0.798173	-0.042884	8	-2.186550	-0.926235	-0.017967				
1	1.513288	0.071659	1.573996	1	1.334198	0.031950	1.569073				
1	-1.500362	1.825575	-0.562570	1	-1.506214	1.825647	-0.556561				
6	2.289211	-0.632657	-0.348433	6	2.146403	-0.681612	-0.328572				
1	3.204202	-0.035262	-0.339028	1	3.088180	-0.146461	-0.262251				
1	2.533968	-1.628912	0.027083	1	2.299615	-1.691058	0.035542				

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	1.952052	-0.722827	-1.382940	1	1.847068	-0.717262	-1.369030				
1	0.169877	-0.734775	0.521554	1	-0.003235	-0.759240	0.495330				
									TS9 G3		
								6	1.612817	0.273984	0.421807
								6	0.547488	0.888027	-0.034041
								6	-0.611372	1.348699	-0.355389
								6	-1.855746	-0.246320	0.478756
								8	-2.370818	-0.981065	-0.200258
								1	2.102260	0.678863	1.293718
								1	-0.776087	2.145372	-1.061854
								6	2.260413	-0.917534	-0.240348
								1	3.265956	-0.679825	-0.578248
								1	2.344753	-1.752537	0.451125
								1	1.687091	-1.246164	-1.099150
								1	-1.379034	0.621672	0.971757
	TS10 CBS-QB3				TS10 CBS-APNO				TS10 G3		
6	-1.584641	0.766631	-0.103169	6	-1.585216	0.740628	-0.100551	6	-1.587954	0.737818	-0.100494
6	-0.191681	1.181764	-0.001408	6	-0.177568	1.174452	-0.004005	6	-0.180687	1.173690	-0.003989
6	0.627957	0.095855	-0.009750	6	0.620162	0.104475	-0.008923	6	0.621451	0.106684	-0.008353
8	-0.096757	-1.059820	-0.009355	8	-0.112521	-1.035963	-0.010504	8	-0.111809	-1.038024	-0.008308
1	0.149876	2.206750	0.025168	1	0.154573	2.192549	0.008990	1	0.148085	2.193146	0.010172
6	2.105754	-0.063196	0.010000	6	2.096820	-0.074262	0.012775	6	2.099307	-0.072374	0.012137
1	2.423430	-0.612557	0.900938	1	2.395793	-0.629809	0.895864	1	2.402367	-0.628784	0.892821
1	2.445486	-0.627912	-0.862873	1	2.421277	-0.631995	-0.859776	1	2.426984	-0.627075	-0.860703
1	2.590810	0.913004	0.008031	1	2.588836	0.889491	0.018674	1	2.591767	0.890925	0.019860
6	-1.429988	-0.636307	-0.024082	6	-1.403574	-0.637519	-0.036825	6	-1.402355	-0.637724	-0.038406
1	-1.863160	-0.036125	0.987235	1	-1.844366	0.050167	0.980992	1	-1.856904	0.058994	0.973001
1	-2.136782	-1.433083	-0.213205	1	-2.119693	-1.429340	-0.135536	1	-2.116394	-1.431570	-0.134052
	TS11 CBS-QB3								TS11 G3		
6	-1.528570	0.865155	0.000086					6	1.506331	0.860193	0.000004
6	-0.187839	1.185019	-0.000030					6	0.189693	1.162642	0.000005
6	0.620938	0.011721	-0.000090					6	-0.627405	-0.030328	-0.000001
8	-0.013372	-1.100113	-0.000020					8	-0.045296	-1.120422	-0.000012
1	0.247116	2.177808	-0.000044					1	-0.250169	2.142441	0.000009

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	2.113095	-0.035589	0.000000					6	-2.127411	-0.007068	0.000002
1	2.465110	-0.579283	0.880732					1	-2.490658	-0.534591	-0.874826
1	2.465246	-0.582298	-0.878784					1	-2.490648	-0.534504	0.874887
1	2.541908	0.966450	-0.001588					1	-2.516093	1.002377	-0.000043
6	-1.619226	-0.548554	-0.000011					6	1.729681	-0.506329	0.000001
1	-2.001074	-1.024264	0.903403					1	2.042307	-0.993499	-0.906545
1	-2.001715	-1.024025	-0.903289					1	2.042291	-0.993503	0.906549
	TS12 CBS-QB3				TS12 CBS-APNO				TS12 G3		
6	-1.727762	1.089712	-0.192852	6	-1.715724	1.087987	-0.176909	6	-1.710658	1.094231	-0.172896
1	-1.874376	1.621045	0.752786	1	-1.857499	1.599275	0.771077	1	-1.864375	1.599714	0.776075
1	-1.124477	1.743451	-0.830499	1	-1.118728	1.739823	-0.807897	1	-1.109305	1.752446	-0.792534
1	-2.689104	0.890240	-0.665797	1	-2.672701	0.895600	-0.642981	1	-2.663297	0.909160	-0.650179
6	-0.985571	-0.206849	0.043317	6	-0.978767	-0.210836	0.040174	6	-0.978800	-0.208957	0.041280
8	-1.401175	-1.278933	-0.317682	8	-1.397804	-1.254276	-0.328012	8	-1.406794	-1.252871	-0.334180
6	0.330753	-0.085917	0.800302	6	0.331901	-0.111636	0.791495	6	0.331467	-0.121182	0.791890
1	0.260973	-0.119960	1.886239	1	0.278561	-0.165036	1.867474	1	0.277380	-0.187419	1.866939
6	1.484948	0.025719	0.210186	6	1.474819	0.017958	0.202342	6	1.476784	0.012493	0.203498
6	2.628768	0.133810	-0.404760	6	2.613279	0.144743	-0.399218	6	2.615436	0.147042	-0.399278
1	3.056729	1.103501	-0.639189	1	3.024477	1.116581	-0.609223	1	3.028949	1.119743	-0.598970
1	3.192852	-0.745661	-0.699240	1	3.175279	-0.721328	-0.701657	1	3.179619	-0.712434	-0.714854
	TS13 CBS-QB3				TS13 CBS-APNO				TS13 G3		
6	-1.384114	-0.775515	0.030655	6	-1.403979	-0.718343	0.011160	6	-1.381226	-0.759365	0.013083
6	-2.068624	0.403747	-0.217842	6	-2.099738	0.461801	-0.134043	6	-2.096495	0.414716	-0.109654
1	-2.720221	0.784665	0.567813	1	-2.687054	0.800316	0.706079	1	-2.677344	0.737602	0.741200
6	-0.302622	-1.350423	0.234936	6	-0.415752	-1.422301	0.145573	6	-0.333771	-1.387556	0.119881
1	0.243628	-2.257964	0.384817	1	0.058775	-2.365690	0.241341	1	0.194821	-2.304420	0.198549
6	1.169702	0.194778	0.013681	6	1.248667	0.202902	-0.002307	6	1.196639	0.203024	0.001770
6	0.507419	1.393526	0.213296	6	0.541761	1.396076	0.136342	6	0.510985	1.411554	0.108556
1	-0.904367	1.100375	-0.135224	1	-0.773244	1.134816	-0.053267	1	-0.862991	1.118336	-0.058726
1	0.311936	1.637407	1.253705	1	0.590501	1.753181	1.154776	1	0.537543	1.813612	1.109655
1	0.870493	2.212447	-0.399951	1	0.857438	2.114830	-0.605076	1	0.782737	2.105884	-0.670459
8	2.142471	-0.402458	-0.262436	8	2.157329	-0.453479	-0.160315	8	2.150395	-0.423459	-0.132148
1	-2.471805	0.546057	-1.220030	1	-2.530799	0.669562	-1.101684	1	-2.554712	0.622420	-1.064854
	TS14 CBS-QB3										

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	-0.968845	0.265473	-0.089454								
6	0.014368	1.212190	-0.092206								
6	1.334832	0.791470	0.088533								
6	1.442017	-0.615412	0.066503								
8	0.401306	-1.303749	-0.082349								
1	-0.234530	2.233565	-0.362846								
1	2.184318	1.456356	0.146631								
6	-2.184970	-0.204804	0.085556								
1	-2.509789	-1.123799	-0.388869								
1	-2.883413	0.293743	0.752899								
1	2.408554	-1.123379	0.157378								
	TS15 CBS-QB3				TS15 CBS-APNO						
6	-0.839295	1.005081	-0.096718	6	-0.809649	1.016674	-0.110765				
6	0.618519	1.116878	-0.077298	6	0.631532	1.129029	-0.067146				
6	-1.492574	-0.159238	-0.019548	6	-1.489681	-0.147696	0.056184				
6	1.492049	0.138309	-0.002367	6	1.491273	0.119210	-0.018858				
6	2.358974	-0.828150	0.078859	6	2.330753	-0.874515	0.044317				
8	-1.934791	-1.226010	-0.113469	8	-2.024080	-1.129730	-0.174971				
1	-2.373398	0.640179	1.641012	1	-1.719111	0.154053	2.007357				
1	-1.444764	1.898957	-0.131115	1	-1.420063	1.899418	-0.091531				
1	2.727318	-1.184533	1.038075	1	2.666614	-1.264583	0.991570				
1	2.750341	-1.319792	-0.808690	1	2.716440	-1.338779	-0.848885				
1	0.992797	2.135983	-0.129101	1	1.023391	2.131512	-0.081138				
	TS16 CBS-QB3				TS16 CBS-APNO				TS16 G3		
6	0.820775	1.026572	0.037963	6	0.834311	1.024752	0.032689	6	0.837487	1.025955	0.035895
6	-0.558870	1.135471	-0.151981	6	-0.546952	1.154209	-0.150606	6	-0.543852	1.157464	-0.151912
6	1.505555	-0.248210	0.410200	6	1.500702	-0.262722	0.402362	6	1.497253	-0.264050	0.405432
6	-1.454712	0.135061	-0.033960	6	-1.450138	0.150497	-0.012980	6	-1.449674	0.151947	-0.018520
6	-2.321368	-0.826853	0.055540	6	-2.308902	-0.830335	0.049862	6	-2.311938	-0.829962	0.051164
8	1.915288	-1.052811	-0.388063	8	1.873945	-1.061918	-0.384017	8	1.875174	-1.064853	-0.386116
1	1.639234	-0.420722	1.502364	1	1.649699	-0.430451	1.476272	1	1.637703	-0.439592	1.476230
1	1.447123	1.905408	-0.074960	1	1.468974	1.887270	-0.074335	1	1.473576	1.887239	-0.069721
1	-2.578998	-1.446151	-0.802696	1	-2.539903	-1.429228	-0.817447	1	-2.548729	-1.433743	-0.810368
1	-2.825687	-1.063335	0.991453	1	-2.814773	-1.078521	0.969775	1	-2.816657	-1.075533	0.971857

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-0.952259	2.115046	-0.418229	1	-0.929681	2.127866	-0.410088	1	-0.922941	2.132335	-0.411429
	TS17 CBS-QB3				TS17 CBS-APNO				TS17 G3		
6	-0.783101	1.060567	0.067026	6	-0.776909	1.037001	0.000000	6	0.779308	1.034894	0.000106
6	0.580295	1.119013	-0.047036	6	0.588065	1.044780	-0.000001	6	-0.589386	1.046475	-0.000009
6	-1.246172	-0.299661	-0.099359	6	-1.289347	-0.342308	-0.000001	6	1.289595	-0.344290	0.000182
6	1.220324	-0.136748	-0.165408	6	1.194917	-0.255099	-0.000002	6	-1.199381	-0.251153	-0.000052
6	2.363723	-0.742450	0.101143	6	2.486368	-0.651055	0.000002	6	-2.492093	-0.652351	-0.000006
8	-2.264526	-0.887463	0.091836	8	-2.369434	-0.782825	0.000001	8	2.378038	-0.781869	-0.000203
1	-0.077769	-0.837790	-0.401194	1	-0.061360	-0.958377	0.000000	1	0.053252	-0.958927	0.000479
1	-1.457962	1.895865	0.195681	1	-1.419340	1.897046	0.000009	1	1.422671	1.893693	0.000226
1	3.147054	-0.258728	0.684688	1	3.295395	0.064939	0.000002	1	-3.304913	0.058071	-0.000753
1	2.564766	-1.756936	-0.228262	1	2.752972	-1.692888	0.000001	1	-2.756109	-1.694312	0.000606
1	1.129701	2.052973	-0.123802	1	1.169241	1.951969	-0.000001	1	-1.167466	1.954980	-0.000254
	TS18 CBS-QB3								TS18 G3		
6	-0.674268	0.435145	-0.085112					6	-0.683837	0.434998	-0.084008
6	0.504473	-0.241308	-0.102548					6	0.506536	-0.244230	-0.085231
6	-1.945236	-0.203152	-0.227393					6	-1.954466	-0.243181	-0.236984
6	1.794745	0.387086	0.017245					6	1.785705	0.394528	0.018000
6	2.954381	-0.286711	0.090840					6	2.963809	-0.282826	0.083116
8	-3.035362	-0.134504	0.223057					8	-3.022369	-0.111936	0.224223
1	1.808139	1.474373	0.046941					1	1.799275	1.471652	0.044782
1	-0.695069	1.525219	-0.057462					1	-0.711836	1.512979	-0.095034
1	2.980788	-1.371364	0.076500					1	2.996242	-1.357884	0.064007
1	3.904297	0.226955	0.170514					1	3.902749	0.233321	0.156478
1	0.480179	-1.325510	-0.179139					1	0.486040	-1.320315	-0.133372
	TS19 CBS-QB3										
6	-0.384860	0.691451	0.000023								
6	0.675530	-0.089781	0.000006								
6	-2.469957	-0.619058	-0.000032								
6	2.064918	0.375933	0.000015								
6	3.118974	-0.445234	-0.000005								
8	-3.413227	0.009497	-0.000010								
1	2.218718	1.451628	0.000038								
1	-0.598790	1.751076	0.000046								

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.997802	-1.523718	-0.000028								
1	4.133268	-0.064722	0.000002								
1	0.527190	-1.170111	-0.000018								
	TS20 CBS-QB3				TS20 CBS-APNO				TS20 G3		
6	0.761935	1.026456	-0.159361	6	0.786833	1.023852	-0.153915	6	0.781512	1.030878	-0.155310
6	-0.639761	1.109800	0.015388	6	-0.628703	1.112856	0.007226	6	-0.632852	1.114813	0.013268
6	1.509784	-0.076945	-0.029504	6	1.505000	-0.089101	-0.030699	6	1.502614	-0.085116	-0.034325
6	-1.461859	-0.028212	0.470237	6	-1.454627	-0.027494	0.470572	6	-1.452832	-0.030997	0.473640
6	-2.081525	-0.890939	-0.333537	6	-2.080070	-0.873410	-0.331780	6	-2.075988	-0.878279	-0.334114
8	2.185406	-1.019397	0.069379	8	2.145978	-1.028037	0.066836	8	2.151190	-1.029730	0.068059
1	-1.560704	-0.165378	1.550566	1	-1.537676	-0.165653	1.540488	1	-1.532808	-0.175434	1.542167
1	1.335212	1.908071	-0.432279	1	1.368979	1.890729	-0.410971	1	1.358615	1.899823	-0.416862
1	-2.021313	-0.803996	-1.413564	1	-2.029051	-0.779830	-1.403375	1	-2.028105	-0.780063	-1.404635
1	-2.671623	-1.709514	0.064818	1	-2.665207	-1.686517	0.061422	1	-2.655903	-1.697355	0.052608
1	-1.096264	2.085024	-0.103904	1	-1.075473	2.085344	-0.090681	1	-1.086044	2.083078	-0.096712
	TS21 CBS-QB3				TS21 CBS-APNO						
6	-0.212922	-1.171084	0.114064	6	0.285901	1.142892	0.102396				
6	1.165193	-0.962101	0.014956	6	-1.080042	1.033769	0.037936				
6	-1.069909	-0.098162	-0.101473	6	1.043906	-0.091024	-0.149474				
6	1.580872	0.367602	-0.131323	6	-1.614458	-0.269352	-0.134944				
6	0.663361	1.363884	0.172111	6	-0.770621	-1.362336	0.170573				
8	-2.162076	0.335776	-0.106592	8	2.182470	-0.320680	-0.074574				
1	2.521140	0.593587	-0.625775	1	-2.539921	-0.407159	-0.667166				
1	-0.670566	-2.144697	0.251382	1	0.813691	2.068612	0.248111				
1	0.083783	1.299801	1.087532	1	-0.295732	-1.411667	1.135144				
1	0.752351	2.363619	-0.238769	1	-0.916987	-2.314158	-0.311360				
1	1.850327	-1.799351	-0.031649	1	-1.708921	1.906121	0.032941				
	TS22 CBS-QB3				TS22 CBS-APNO				TS22 G3		
6	-0.112041	-1.236518	0.087725	6	-0.093839	-1.218780	0.083269	6	-0.094435	-1.219312	0.083863
6	-1.364350	-0.768663	0.038748	6	-1.380409	-0.746071	0.026386	6	-1.383617	-0.745163	0.028891
6	0.819151	-0.055951	-0.052378	6	0.833535	-0.052936	-0.041844	6	0.831932	-0.053885	-0.043736
6	-1.346168	0.720020	-0.130731	6	-1.369940	0.697683	-0.119793	6	-1.371768	0.697583	-0.119973
6	-0.079683	1.157901	-0.167520	6	-0.065451	1.151889	-0.121326	6	-0.065008	1.150382	-0.128472
8	2.025137	-0.076032	-0.082605	8	2.015725	-0.072941	-0.090182	8	2.020240	-0.074460	-0.088706

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-2.242405	1.320988	-0.207424	1	-2.250023	1.305059	-0.202082	1	-2.251050	1.306113	-0.200709
1	0.229951	-2.253809	0.203586	1	0.236377	-2.232925	0.185545	1	0.235725	-2.233071	0.187742
1	0.288784	2.161104	-0.316906	1	0.287350	2.143942	-0.317680	1	0.288958	2.142328	-0.321947
1	0.297303	1.826164	2.219187	1	0.329724	1.716484	2.018076	1	0.337763	1.740659	2.037829
1	-2.276181	-1.346923	0.107333	1	-2.272600	-1.339753	0.077450	1	-2.275937	-1.337984	0.083293
	TS23a CBS-QB3				TS23a CBS-APNO				TS23a G3		
6	0.109750	1.188630	-0.032731	6	0.098830	1.177958	-0.047201	6	0.102000	1.175739	-0.047813
6	1.456409	0.806805	-0.111312	6	1.425670	0.815279	-0.108481	6	1.428242	0.814214	-0.106479
6	-0.820504	-0.039991	-0.009311	6	-0.818745	-0.045990	-0.008857	6	-0.817638	-0.045489	-0.010664
6	1.379787	-0.714904	0.007431	6	1.364624	-0.709745	0.004006	6	1.364422	-0.710283	0.003639
6	0.128096	-1.192826	-0.003311	6	0.132053	-1.192288	0.001815	6	0.130598	-1.193334	0.002329
8	-2.025271	-0.043901	0.007078	8	-1.998013	-0.040391	0.009473	8	-2.002779	-0.037003	0.010991
1	2.281510	-1.312615	0.053996	1	2.262841	-1.296730	0.036654	1	2.261578	-1.298432	0.037298
1	-0.270913	2.192986	-0.195450	1	-0.285726	2.179869	-0.128502	1	-0.283216	2.177008	-0.131377
1	-0.204097	-2.221598	0.027058	1	-0.186708	-2.215600	0.032769	1	-0.189107	-2.216213	0.030156
1	0.874433	1.406141	0.953183	1	0.979112	1.384303	0.935604	1	0.987228	1.388583	0.929919
	TS23b CBS-QB3				TS23b CBS-APNO				TS23b G3		
6	0.229503	1.381528	0.212423	6	0.406138	1.406143	0.269881	6	0.418465	1.409991	0.259309
6	1.288316	0.709316	-0.379869	6	1.276552	0.631537	-0.445855	6	1.293269	0.620071	-0.434960
6	-0.835093	-0.221125	0.038887	6	-0.882982	-0.220614	0.024483	6	-0.886825	-0.216993	0.025885
6	1.432833	-0.612865	-0.007699	6	1.339111	-0.702423	-0.044656	6	1.339961	-0.710968	-0.039493
6	0.170550	-1.210631	0.113213	6	0.085856	-1.230800	0.166133	6	0.075801	-1.231326	0.157679
8	-1.988775	-0.059257	-0.148577	8	-1.964272	0.074366	-0.178218	8	-1.976986	0.082735	-0.172072
1	2.371508	-1.147705	0.069976	1	2.242139	-1.284280	-0.002226	1	2.235258	-1.303393	0.009234
1	-0.263383	2.223936	-0.266176	1	0.000329	2.322202	-0.128330	1	0.020020	2.320631	-0.157226
1	-0.071725	-2.260263	0.219626	1	-0.206604	-2.238499	0.388877	1	-0.220900	-2.238988	0.375798
1	0.157146	1.380751	1.303462	1	0.330267	1.302589	1.347496	1	0.337484	1.335221	1.338246
	TS24 CBS-QB3				TS24 CBS-APNO				TS24 G3		
6	1.560099	0.615001	-0.068495	6	1.556558	0.609942	-0.076281	6	1.557922	0.610937	-0.078462
6	0.244748	1.160611	-0.034851	6	0.245794	1.161286	-0.022532	6	0.248856	1.162348	-0.019784
6	-0.627574	0.096936	0.057045	6	-0.622869	0.091619	0.102604	6	-0.623889	0.092289	0.110429
8	0.090747	-1.070399	0.010240	8	0.089573	-1.059687	0.016042	8	0.089413	-1.062042	0.019849
6	1.409155	-0.736584	-0.035749	6	1.396847	-0.735937	-0.043732	6	1.398697	-0.737358	-0.045442
1	2.493181	1.154249	-0.103039	1	2.486511	1.137307	-0.126023	1	2.487226	1.139659	-0.131518

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-0.033918	2.202430	-0.038178	1	-0.031635	2.195110	-0.020150	1	-0.026713	2.196919	-0.017239
6	-2.100786	-0.023743	-0.144085	6	-2.089195	-0.020055	-0.164886	6	-2.088930	-0.019192	-0.171924
1	-2.516366	-0.817867	0.477970	1	-2.526436	-0.821304	0.417544	1	-2.530949	-0.827501	0.396216
1	-2.591193	0.914164	0.119190	1	-2.585981	0.908058	0.090290	1	-2.590749	0.903775	0.090645
1	-2.329875	-0.252803	-1.190366	1	-2.262170	-0.229175	-1.217612	1	-2.256435	-0.214994	-1.227528
1	-0.764431	0.249922	2.038767	1	-0.809244	0.195236	2.009568	1	-0.842966	0.196134	2.017384
1	2.102776	-1.560229	-0.029442	1	2.089562	-1.548865	-0.052990	1	2.089337	-1.551806	-0.055651
	TS25 CBS-QB3				TS25 CBS-APNO				TS25 G3		
6	0.349216	1.175192	0.316862	6	0.339650	1.172493	0.320714	6	0.342482	1.171970	0.321992
6	1.400848	0.612548	-0.454401	6	1.400693	0.619224	-0.437144	6	1.402850	0.621515	-0.439705
6	1.276936	-0.741991	-0.347876	6	1.274943	-0.734623	-0.340741	6	1.280085	-0.733665	-0.344921
8	0.219259	-1.067889	0.446084	8	0.218811	-1.066630	0.431171	8	0.223986	-1.068601	0.430168
1	0.132545	2.220145	0.470502	1	0.113353	2.206903	0.477219	1	0.116174	2.206293	0.479944
1	2.157011	1.139974	-1.014275	1	2.159887	1.144623	-0.979180	1	2.158437	1.150607	-0.983544
6	-0.405652	0.109576	0.784857	6	-0.431570	0.087959	0.759496	6	-0.425443	0.086865	0.762844
1	-1.076098	0.043827	1.625074	1	-1.048223	0.027637	1.631043	1	-1.042072	0.022058	1.633596
6	-2.230310	-0.018315	-0.590883	6	-2.199982	-0.011771	-0.580707	6	-2.216484	-0.011260	-0.578300
1	-2.669836	-0.941066	-0.230231	1	-2.649958	-0.927124	-0.232851	1	-2.670367	-0.921118	-0.224005
1	-2.774677	0.895640	-0.383439	1	-2.758775	0.889906	-0.388246	1	-2.767889	0.894296	-0.388068
1	-1.703680	-0.067592	-1.535703	1	-1.711727	-0.065932	-1.538946	1	-1.732084	-0.073279	-1.536954
1	1.834440	-1.569885	-0.751959	1	1.842558	-1.542668	-0.748115	1	1.844983	-1.542599	-0.753770
	TS26 CBS-QB3				TS26 G3						
6	-1.306511	-0.705208	0.135840	6	-1.291456	-0.703114	0.128444				
6	-1.305314	0.677794	0.380340	6	-1.287546	0.669431	0.391810				
6	-0.178395	1.271876	-0.183958	6	-0.178552	1.271572	-0.182628				
6	0.874747	0.365088	-0.507263	6	0.884754	0.386620	-0.500308				
8	-0.291940	-1.242020	-0.426007	8	-0.305435	-1.229019	-0.441411				
1	-2.171150	1.207964	0.753084	1	-2.145851	1.193013	0.765917				
1	-0.198207	2.279189	-0.589064	1	-0.197672	2.269854	-0.585630				
6	1.809937	-0.216005	0.520334	6	1.791028	-0.237480	0.522730				
1	2.200198	-1.182049	0.193997	1	2.167182	-1.189938	0.174113				
1	2.658763	0.467447	0.646119	1	2.637549	0.430494	0.673038				
1	1.318874	-0.332396	1.486721	1	1.285542	-0.371877	1.468012				
1	1.332248	0.474227	-1.492875	1	1.341175	0.498636	-1.472775				

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-2.171980	-1.339495	0.338313	1	-2.153813	-1.320200	0.348326				
	TS27 CBS-QB3										
6	-1.429927	-0.109874	0.386499								
6	-0.625843	1.120929	0.119731								
6	0.738657	1.204035	-0.101520								
6	1.683487	0.184046	-0.119625								
8	-1.979509	-0.759587	-0.468800								
1	-1.213022	2.035720	0.096116								
1	1.120188	2.204553	-0.289928								
6	1.420127	-1.274642	0.100980								
1	2.342125	-1.853529	0.030198								
1	0.988811	-1.468879	1.090931								
1	0.712921	-1.675823	-0.632913								
1	2.708750	0.476731	-0.319730								
1	-1.542714	-0.389042	1.459332								
	TS28 CBS-QB3				TS28 CBS-APNO						
6	-1.222954	-0.218449	0.204094	6	-1.314210	-0.341614	0.030707				
6	-0.751725	1.057354	-0.321867	6	-0.830465	1.035831	-0.186037				
6	0.550719	1.247869	0.001858	6	0.470546	1.123697	0.071519				
6	1.237514	0.072884	0.553718	6	1.152755	-0.126687	0.532647				
8	-2.177769	-0.906033	0.011215	8	-2.371994	-0.828473	-0.046168				
1	-1.415993	1.766995	-0.798947	1	-1.471204	1.832954	-0.515374				
1	1.040441	2.215146	-0.083948	1	1.021992	2.043465	-0.050768				
6	1.848427	-0.959421	-0.377159	6	2.263981	-0.667917	-0.342129				
1	2.794827	-0.599871	-0.800641	1	3.114190	0.013422	-0.370435				
1	2.065188	-1.886899	0.160610	1	2.618487	-1.621151	0.034987				
1	1.181265	-1.192803	-1.210194	1	1.923769	-0.812953	-1.362938				
1	1.856727	0.268695	1.432265	1	1.389822	-0.119836	1.589528				
1	-0.072187	-0.524421	0.847263	1	-0.076744	-0.847972	0.404098				
	TS29 CBS-QB3										
6	-2.018042	-0.711661	0.130445								
6	-0.504868	1.178151	-0.151892								
6	0.770363	1.021332	0.098123								
6	1.460828	-0.235204	0.569801								

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
8	-3.085693	-0.424933	-0.126511								
1	-1.145314	1.980228	-0.489748								
1	1.428877	1.885953	-0.060285								
6	2.520460	-0.729586	-0.426106								
1	3.280273	0.035418	-0.612533								
1	3.028469	-1.617676	-0.041212								
1	2.063915	-0.988054	-1.384849								
1	1.943461	-0.024562	1.532006								
1	0.713418	-1.010035	0.746480								
	TS30 CBS-QB3				TS30 G3						
6	-1.540780	-0.539698	-0.100830	6	-1.546785	-0.522057	-0.069520				
6	-1.384277	0.847040	-0.021764	6	-1.368667	0.851126	-0.007142				
6	-0.028732	1.182549	0.055338	6	-0.007977	1.174081	0.014195				
6	0.810595	0.085147	0.398168	6	0.815658	0.098782	0.395795				
8	-0.499807	-1.290908	-0.007471	8	-0.536838	-1.285350	-0.065227				
1	-2.194285	1.542425	-0.194202	1	-2.170293	1.551750	-0.139918				
1	0.374605	2.101120	-0.359811	1	0.400595	2.049833	-0.460216				
1	-2.495086	-1.025321	-0.308681	1	-2.525378	-0.974655	-0.157641				
6	2.155175	-0.136571	-0.225491	6	2.171314	-0.155230	-0.187141				
1	2.936040	0.337887	0.382509	1	2.938678	0.215978	0.488416				
1	2.378985	-1.204975	-0.257734	1	2.320209	-1.222527	-0.296789				
1	2.207413	0.264049	-1.238898	1	2.291925	0.316987	-1.153460				
1	0.718902	-0.318721	1.404064	1	0.657711	-0.334774	1.364297				
	TS31 CBS-QB3				TS31 CBS-APNO				TS31 G3		
6	-1.789434	-0.106507	0.385294	6	-1.789811	-0.121111	0.380522	6	-1.789197	-0.120293	0.383494
6	-0.861835	0.994974	-0.010633	6	-0.869931	0.991890	-0.007508	6	-0.870709	0.992520	-0.005861
6	0.514233	0.851886	-0.108996	6	0.512956	0.856215	-0.104444	6	0.513168	0.856162	-0.105336
6	1.228006	-0.317769	0.090682	6	1.225616	-0.319551	0.090129	6	1.227069	-0.320490	0.089902
8	-2.326808	-0.859165	-0.389190	8	-2.319272	-0.847499	-0.388132	8	-2.324580	-0.847185	-0.389864
1	-1.323145	1.959633	-0.200215	1	-1.332436	1.947748	-0.185846	1	-1.332375	1.947916	-0.187262
1	1.081743	1.742849	-0.371660	1	1.070270	1.744109	-0.357246	1	1.070150	1.743191	-0.359899
1	-1.984381	-0.196878	1.479199	1	-1.974237	-0.230938	1.457379	1	-1.969059	-0.236486	1.457266
6	2.712774	-0.424167	-0.019667	6	2.717597	-0.421712	-0.021644	6	2.719843	-0.421773	-0.022131
1	3.158349	-0.780040	0.917710	1	3.001296	-1.126896	-0.799567	1	3.160239	-0.774106	0.907505

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	3.003016	-1.149015	-0.790453	1	3.165650	0.537728	-0.257307	1	3.006215	-1.128662	-0.796877
1	3.170781	0.536068	-0.268462	1	3.155169	-0.779006	0.907882	1	3.167390	0.536687	-0.261732
1	0.685639	-1.229796	0.327316	1	0.689905	-1.227142	0.317436	1	0.693037	-1.227820	0.319502
	TS32 CBS-QB3										
6	1.354530	-0.306027	-0.123194								
6	0.871326	1.061377	-0.066046								
6	-0.481112	1.084587	0.071243								
6	-1.093662	-0.203245	0.388083								
8	2.414358	-0.842382	-0.014152								
1	1.527262	1.910100	-0.212404								
1	-1.078231	1.974256	-0.114694								
1	0.119327	-0.880455	-0.072224								
6	-2.417510	-0.584398	-0.229180								
1	-2.647428	-1.636783	-0.047567								
1	-3.238135	0.004758	0.202869								
1	-2.424159	-0.417507	-1.309075								
1	-0.974931	-0.529072	1.420874								
	TS33 CBS-QB3										
6	-1.760847	-0.153546	0.350781								
6	-0.644087	0.693204	0.660108								
6	0.426824	1.000924	-0.299911								
6	1.572933	0.334937	-0.444210								
8	-1.911146	-0.730548	-0.724751								
1	-0.636165	1.167963	1.640345								
1	0.238569	1.858745	-0.946480								
6	1.999213	-0.876288	0.329414								
1	2.129346	-1.733075	-0.340407								
1	2.964895	-0.708195	0.818375								
1	1.270552	-1.155093	1.093029								
1	2.268204	0.686894	-1.202466								
1	-2.510445	-0.268244	1.158525								
	TS34 CBS-QB3								TS34 G3		
6	1.663473	-0.354916	0.222031					6	1.662469	-0.364979	0.208758
6	0.339737	-0.104890	0.827974					6	0.348910	-0.116115	0.829707

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	-0.520710	0.998048	0.287384					6	-0.511449	0.988116	0.295185
6	-1.647123	0.555590	-0.271156					6	-1.630038	0.565740	-0.264609
8	2.036263	0.118935	-0.831631					8	2.023564	0.127065	-0.824837
1	0.331430	-0.244944	1.912694					1	0.348873	-0.254314	1.903774
1	-0.227771	2.039385	0.352111					1	-0.220155	2.019952	0.373378
6	-1.775209	-0.929609	-0.273272					6	-1.784500	-0.921159	-0.275439
1	-2.549887	-1.387615	0.341467					1	-2.553847	-1.351256	0.350217
1	-1.606350	-1.451698	-1.215120					1	-1.684879	-1.421040	-1.228528
1	-0.502958	-1.040260	0.408624					1	-0.528987	-1.072198	0.387558
1	-2.410925	1.198621	-0.698314					1	-2.374032	1.216960	-0.689835
1	2.315352	-1.050298	0.793813					1	2.312157	-1.064243	0.740527
	TS35 CBS-QB3				TS35 CBS-APNO				TS35 G3		
6	-1.718519	-0.067883	-0.012819	6	-1.734754	-0.048217	-0.031313	6	-1.732961	-0.053512	-0.028654
6	-0.674954	0.910584	0.543122	6	-0.673887	0.858003	0.579517	6	-0.679685	0.863953	0.576314
6	0.544796	1.078284	-0.313228	6	0.530899	1.062919	-0.303166	6	0.526878	1.066694	-0.305637
6	1.636654	0.218718	-0.331604	6	1.650729	0.235485	-0.348860	6	1.646375	0.236682	-0.348753
8	-1.470669	-1.176429	-0.403254	8	-1.529566	-1.155444	-0.386429	8	-1.512103	-1.162202	-0.389497
1	-0.401589	0.518442	1.532825	1	-0.384293	0.405719	1.524421	1	-0.389022	0.422908	1.526055
1	0.557236	1.938749	-0.973215	1	0.511059	1.921935	-0.951465	1	0.506290	1.923493	-0.956125
6	1.779568	-0.950134	0.386200	6	1.842331	-0.938968	0.364773	6	1.837661	-0.936308	0.369829
1	0.987726	-1.337546	1.014089	1	1.083664	-1.350196	1.003559	1	1.079287	-1.346362	1.008884
1	2.684439	-1.539593	0.311992	1	2.756692	-1.494293	0.263847	1	2.750545	-1.493729	0.272362
1	2.458966	0.506107	-0.983189	1	2.443944	0.546075	-1.009869	1	2.440575	0.544557	-1.009197
1	-2.764365	0.312399	-0.013675	1	-2.742063	0.380821	-0.114009	1	-2.744678	0.358781	-0.103661
1	-1.162331	1.875452	0.707182	1	-1.124381	1.818156	0.809244	1	-1.135781	1.822909	0.799065
	TS36 CBS-QB3										
6	-1.866936	0.110186	-0.283793								
6	-0.108861	1.329075	0.673249								
6	0.825789	1.066785	-0.276498								
6	1.651235	-0.129325	-0.367114								
8	-1.905692	-1.042099	-0.031326								
1	-0.203609	0.719879	1.563700								
1	0.968277	1.799316	-1.067286								
6	1.468424	-1.276578	0.303623								

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	0.642055	-1.423370	0.989005								
1	2.139728	-2.115241	0.163669								
1	2.477193	-0.072073	-1.071933								
1	-1.964428	0.550278	-1.308153								
1	-0.631588	2.277147	0.684802								
	TS37 CBS-QB3										
6	-1.550008	-0.002934	0.036896								
6	-0.741341	1.132676	0.208104								
6	0.631668	1.260258	-0.069612								
6	1.544873	0.214872	-0.193587								
8	-1.208500	-1.195080	-0.282647								
1	-1.298733	2.046200	0.386334								
1	0.995897	2.266824	-0.258181								
6	1.302072	-1.100905	0.280542								
1	2.042549	-1.859454	0.044467								
1	0.932323	-1.174675	1.306633								
1	0.041744	-1.315522	-0.167674								
1	2.461124	0.421493	-0.743010								
1	-2.630485	0.151967	0.118549								
	TS38 CBS-QB3				TS38 CBS-APNO						
6	-1.097354	0.169985	0.429522	6	-1.105615	0.148216	0.464020				
6	-0.152848	1.202977	0.413708	6	-0.174930	1.228529	0.373364				
6	1.057516	0.932042	-0.341674	6	1.061407	0.953743	-0.302279				
6	1.424443	-0.373560	-0.318820	6	1.462646	-0.349583	-0.296457				
8	-1.663375	-0.397867	-0.676839	8	-1.672491	-0.409277	-0.649225				
1	-0.161332	1.929853	1.219730	1	-0.278316	2.090391	1.011608				
1	1.647709	1.704921	-0.823479	1	1.676888	1.738223	-0.707899				
6	0.638854	-1.275214	0.534746	6	0.647405	-1.324001	0.481000				
1	0.812974	-1.214386	1.606687	1	0.996190	-1.550520	1.478090				
1	0.380110	-2.267353	0.174413	1	0.177102	-2.146560	-0.031621				
1	-1.074694	-0.238775	-1.426554	1	-1.125494	-0.246290	-1.398109				
1	2.263250	-0.742093	-0.906002	1	2.385058	-0.656283	-0.762481				
1	-1.784685	0.073388	1.265028	1	-1.796977	0.103835	1.286322				
	TS39 CBS-QB3				TS39 CBS-APNO				TS39 G3		

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	0.070398	0.999075	0.565090	6	0.575854	0.032148	0.750897	6	0.571200	0.032142	0.753582
6	0.524055	-0.266857	0.831382	6	-0.148242	-1.138092	0.462884	6	-0.151462	-1.138795	0.462622
6	-0.413825	-1.231669	0.241849	6	-1.310023	-0.799907	-0.300557	6	-1.312623	-0.801415	-0.302263
6	-1.392736	-0.571250	-0.402495	6	-1.399759	0.561930	-0.429474	6	-1.403050	0.562446	-0.430972
8	2.077345	0.021456	-0.647400	8	2.079469	0.007045	-0.623196	8	2.092296	0.006765	-0.620180
1	1.322128	-0.525391	1.508612	1	0.149222	-2.132288	0.737835	1	0.144551	-2.132870	0.739314
1	-0.299431	-2.305116	0.309406	1	-2.003972	-1.512509	-0.706151	1	-2.004701	-1.514773	-0.709335
6	-1.178306	0.914845	-0.265373	6	-0.258574	1.217493	0.310927	6	-0.261051	1.219091	0.309453
1	-2.024498	1.407325	0.233283	1	-0.626042	1.765096	1.178365	1	-0.626147	1.772481	1.173568
1	-1.072774	1.414924	-1.237318	1	0.307234	1.911859	-0.298829	1	0.306024	1.911073	-0.301701
1	1.479942	-0.135894	-1.394606	1	1.638823	-0.533875	-1.264749	1	1.647134	-0.537924	-1.265811
1	-2.216336	-1.011916	-0.947886	1	-2.163283	1.098886	-0.959200	1	-2.164501	1.100414	-0.962309
1	0.534686	1.919557	0.884988	1	1.306728	0.105044	1.530228	1	1.301196	0.106663	1.533183
	TS40 CBS-QB3				TS40 CBS-APNO				TS40 G3		
6	1.554696	0.560770	-0.101653	6	1.554956	0.549106	-0.097716	6	1.556602	0.548530	-0.096705
6	0.223444	1.130250	-0.103338	6	0.227491	1.136179	-0.085386	6	0.230845	1.137578	-0.083949
6	-0.645423	0.058357	-0.066358	6	-0.642493	0.057958	-0.078488	6	-0.643720	0.058770	-0.079582
8	0.062245	-1.099956	0.063714	8	0.062006	-1.092409	0.063607	8	0.060769	-1.095194	0.063091
6	1.393540	-0.772843	0.027052	6	1.375270	-0.775503	0.023877	6	1.376108	-0.778259	0.024437
1	2.489473	1.095431	-0.147150	1	2.490464	1.066018	-0.143272	1	2.491697	1.066582	-0.143776
1	-0.043578	2.133766	-0.393863	1	-0.030226	2.119588	-0.421557	1	-0.022964	2.118162	-0.432613
6	-2.124257	-0.044164	-0.029922	6	-2.123556	-0.040703	-0.024309	6	-2.126239	-0.039235	-0.023074
1	-2.472155	-0.361962	0.959735	1	-2.453836	-0.353994	0.963509	1	-2.460211	-0.343009	0.965839
1	-2.572193	0.925170	-0.251163	1	-2.568792	0.922243	-0.243695	1	-2.571971	0.921390	-0.250651
1	-2.489161	-0.772916	-0.759260	1	-2.488497	-0.765816	-0.744753	1	-2.494374	-0.769016	-0.736611
1	0.100334	1.786970	1.624616	1	0.144252	1.781331	1.560064	1	0.151487	1.800331	1.552821
1	2.077323	-1.601037	0.102691	1	2.060581	-1.592309	0.092983	1	2.058603	-1.597188	0.093502
	TS41 CBS-QB3				TS41 CBS-APNO				TS41 G3		
6	-0.710083	-0.048086	-0.252725	6	-0.717942	-0.002774	-0.364821	6	-0.719334	-0.000291	-0.366274
6	0.205712	1.144439	-0.284597	6	0.247012	1.155385	-0.371139	6	0.248929	1.156099	-0.373192
6	1.544267	0.575003	0.212119	6	1.478169	0.541367	0.294701	6	1.478059	0.542423	0.295136
6	1.619898	-0.726204	0.278964	6	1.465813	-0.772978	0.366783	6	1.466645	-0.776071	0.368919
8	-0.125018	-1.158688	-0.406024	8	-0.125461	-1.117822	-0.577063	8	-0.127300	-1.120784	-0.580914
1	0.357471	1.540098	-1.298238	1	0.502103	1.481782	-1.376633	1	0.503762	1.482188	-1.378657

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.356300	1.259687	0.440106	1	2.290029	1.156865	0.641483	1	2.286298	1.160646	0.644840
1	-0.170054	1.973352	0.325883	1	-0.134375	2.014582	0.171100	1	-0.131572	2.017102	0.166395
6	-2.086680	0.029651	0.343959	6	-1.962631	0.033722	0.475953	6	-1.962124	0.034593	0.478961
1	-2.693434	0.791302	-0.154139	1	-2.577830	0.892007	0.224554	1	-2.574198	0.897377	0.237497
1	-2.585189	-0.936364	0.265369	1	-2.540111	-0.870662	0.330030	1	-2.545882	-0.864407	0.326215
1	-2.028259	0.307917	1.407250	1	-1.703198	0.108638	1.533482	1	-1.704206	0.097325	1.536815
1	2.324622	-1.515313	0.475646	1	2.104545	-1.568966	0.683627	1	2.111157	-1.564478	0.692913
	TS42 CBS-QB3				TS42 CBS-APNO				TS42 G3		
6	-2.013775	-0.366938	0.577702	6	-2.071419	-0.322483	0.514919	6	-2.080505	-0.314540	0.505247
6	-0.807537	0.152027	-0.178833	6	-0.805745	0.157550	-0.156757	6	-0.803601	0.155182	-0.154562
6	0.280302	-0.871461	-0.515499	6	0.264469	-0.895770	-0.416159	6	0.263028	-0.904386	-0.404032
6	1.656883	-0.510608	0.008315	6	1.672821	-0.513384	-0.026810	6	1.673950	-0.516918	-0.027521
6	2.027924	0.617979	0.552186	6	2.065847	0.621303	0.530176	6	2.065784	0.624947	0.525574
1	2.934243	1.045025	0.953095	1	3.017472	0.994804	0.851035	1	3.020896	0.995707	0.837569
1	2.399893	-1.309318	-0.103793	1	2.417925	-1.274635	-0.225148	1	2.417176	-1.278205	-0.227851
1	0.004200	-1.865292	-0.148936	1	0.000884	-1.825147	0.081448	1	-0.001430	-1.825561	0.108112
1	0.327800	-0.946032	-1.610018	1	0.236132	-1.106304	-1.484949	1	0.228891	-1.134331	-1.468427
8	-0.701774	1.308993	-0.507072	8	-0.663093	1.284924	-0.493108	8	-0.651179	1.286858	-0.491601
1	-2.726105	0.440537	0.740881	1	-2.786274	0.486366	0.574778	1	-2.790135	0.499360	0.554254
1	-1.695907	-0.782727	1.539844	1	-1.838607	-0.682935	1.513712	1	-1.866611	-0.672805	1.508593
1	-2.492721	-1.180133	0.022280	1	-2.498624	-1.154841	-0.038224	1	-2.511295	-1.144745	-0.047679
	TS43 CBS-QB3				TS43 CBS-APNO				TS43 G3		
6	-1.442252	1.212899	-0.141451	6	-1.444569	1.200241	-0.147038	6	-1.431288	1.207248	-0.149593
6	-0.969020	-0.218405	0.029415	6	-0.960971	-0.223366	0.026027	6	-0.958971	-0.220377	0.026580
6	0.371660	-0.441087	0.737631	6	0.367998	-0.440107	0.738632	6	0.365761	-0.447471	0.743634
6	1.516431	0.391904	0.168269	6	1.505277	0.402077	0.187009	6	1.508110	0.395342	0.202116
6	2.519668	-0.076534	-0.507065	6	2.505301	-0.073656	-0.518629	6	2.495008	-0.074895	-0.533056
1	3.348920	-0.463308	-1.051205	1	3.320689	-0.460507	-1.071801	1	3.299112	-0.453928	-1.109348
1	1.446248	1.469165	0.366153	1	1.464677	1.464066	0.401377	1	1.482072	1.450019	0.447979
1	0.235055	-0.171049	1.793541	1	0.218153	-0.186555	1.787643	1	0.213554	-0.205479	1.794876
1	0.596785	-1.505093	0.680035	1	0.600943	-1.493498	0.674464	1	0.595473	-1.501182	0.672002
8	-1.619584	-1.156474	-0.366997	8	-1.597016	-1.145793	-0.364541	8	-1.604849	-1.141317	-0.367835
1	-2.471764	1.213173	-0.496612	1	-2.480897	1.190511	-0.455035	1	-2.465607	1.206343	-0.464059
1	-0.809843	1.725280	-0.873363	1	-0.850658	1.695195	-0.909888	1	-0.831750	1.702174	-0.907630

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-1.367653	1.770965	0.796631	1	-1.334997	1.765996	0.773568	1	-1.325783	1.773506	0.770773
	TS44 CBS-QB3				TS44 CBS-APNO				TS44 G3		
6	-0.889094	0.160016	0.214602	6	-0.908881	0.147902	0.207838	6	-0.915722	0.140185	0.210750
6	0.038263	-0.630202	1.020699	6	0.029562	-0.585411	1.063961	6	0.008601	-0.592059	1.075379
6	1.885440	-0.598981	-0.189644	6	1.911179	-0.550980	-0.114319	6	1.926964	-0.544786	-0.105750
6	2.201396	0.529887	-0.543327	6	2.212390	0.554320	-0.606715	6	2.221988	0.562210	-0.611507
8	-0.910707	1.380684	0.292609	8	-1.020192	1.339765	0.301003	8	-1.032432	1.338518	0.310135
1	0.485037	-0.138151	1.874683	1	0.408972	-0.061409	1.921237	1	0.391385	-0.070776	1.931831
1	2.060176	-1.651782	-0.138684	1	2.228742	-1.559049	0.004841	1	2.254319	-1.548561	0.022546
1	-0.081092	-1.707524	1.077667	1	-0.056736	-1.655763	1.138278	1	-0.062505	-1.663258	1.140453
6	-1.795342	-0.591023	-0.748545	6	-1.703796	-0.646399	-0.804643	6	-1.690616	-0.645426	-0.824813
1	-2.478785	-1.249126	-0.202744	1	-2.365271	-1.343750	-0.297635	1	-2.325892	-1.385559	-0.346926
1	-2.373065	0.123855	-1.332724	1	-2.291198	0.027140	-1.413351	1	-2.303668	0.028599	-1.406864
1	-1.203743	-1.220661	-1.420568	1	-1.037630	-1.224570	-1.437931	1	-1.009937	-1.174684	-1.484688
1	2.233165	1.579733	-0.721208	1	2.031937	1.582683	-0.800193	1	2.008471	1.585345	-0.801791
	TS45 CBS-QB3				TS45 CBS-APNO				TS45 G3		
6	-0.587973	1.358624	0.333214	6	-0.603265	1.357283	0.330694	6	-0.600040	1.359804	0.326771
6	-0.941204	-0.062010	0.051807	6	-0.933508	-0.069774	0.038133	6	-0.933646	-0.067814	0.038035
6	0.154641	-1.071651	0.397148	6	0.154301	-1.072853	0.387656	6	0.152800	-1.074244	0.385005
6	1.525902	-0.604239	-0.062007	6	1.525824	-0.602828	-0.055736	6	1.527273	-0.607628	-0.057358
6	1.803152	0.652662	-0.345243	6	1.787608	0.667644	-0.337333	6	1.794721	0.666900	-0.333306
1	2.713050	1.136639	-0.674932	1	2.707839	1.119233	-0.656012	1	2.716261	1.116636	-0.648631
1	2.292781	-1.374422	-0.153271	1	2.296576	-1.354775	-0.131592	1	2.293170	-1.363216	-0.136407
1	0.171858	-1.229948	1.484361	1	0.154546	-1.230323	1.466379	1	0.151862	-1.236268	1.462950
1	-0.113225	-2.027109	-0.058598	1	-0.102914	-2.017845	-0.074487	1	-0.107210	-2.018085	-0.077895
8	-1.971068	-0.400115	-0.492676	8	-1.949462	-0.404272	-0.482190	8	-1.958805	-0.401997	-0.477385
1	-1.227176	2.085017	-0.163207	1	-1.233767	2.070322	-0.176650	1	-1.223999	2.073983	-0.186205
1	0.613065	1.390999	-0.128739	1	0.642994	1.400653	-0.131829	1	0.652023	1.402195	-0.126299
1	-0.408923	1.579435	1.386277	1	-0.455337	1.570078	1.381234	1	-0.458316	1.578625	1.376690
	TS46 CBS-QB3				TS46 CBS-APNO						
6	-1.355492	1.251425	0.263984	6	-1.517316	1.169571	0.222946				
6	-0.967332	-0.112745	0.038810	6	-0.956075	-0.130496	0.036650				
6	0.248473	-0.674047	0.782419	6	0.259812	-0.565485	0.840499				
6	1.554064	-0.472666	0.030618	6	1.568431	-0.416929	0.081703				

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	2.009721	0.679994	-0.450150	6	2.006302	0.689700	-0.483020				
1	2.957741	0.731553	-0.972804	1	2.951118	0.713710	-0.996522				
1	2.151396	-1.368714	-0.113394	1	2.177741	-1.303518	0.021803				
1	0.322007	-0.223447	1.778367	1	0.313048	-0.008376	1.771229				
1	0.066457	-1.741151	0.916081	1	0.112651	-1.607632	1.095908				
8	-1.606356	-0.821863	-0.742179	8	-1.460273	-0.900150	-0.773618				
1	-2.197239	1.644293	-0.292857	1	-2.367127	1.453409	-0.369624				
1	1.462649	1.612459	-0.351327	1	1.446502	1.610201	-0.464706				
1	-0.848764	1.888150	0.979277	1	-1.118682	1.865240	0.938190				
	TS47 CBS-QB3				TS47 CBS-APNO						
6	1.713315	-0.962611	-0.483350	6	1.839991	-0.874090	-0.552189				
6	1.186107	0.209681	-0.063920	6	1.212304	0.238895	-0.009779				
6	-0.446242	-0.345923	1.040287	6	-0.472863	-0.478222	1.005349				
6	-1.406619	-0.572665	0.009041	6	-1.459828	-0.596873	-0.030745				
6	-2.203031	0.391354	-0.523752	6	-2.219290	0.437873	-0.494131				
1	-2.908199	0.168061	-1.314616	1	-2.925839	0.296626	-1.291795				
1	-1.479639	-1.580331	-0.392699	1	-1.575789	-1.563436	-0.495794				
1	-0.083616	-1.195368	1.603996	1	-0.150068	-1.383110	1.489157				
1	-0.497717	0.584619	1.593322	1	-0.513678	0.387649	1.643312				
8	1.266014	1.394172	-0.002772	8	1.220269	1.399919	0.048198				
1	2.778128	-0.983373	-0.687974	1	2.876909	-1.011713	-0.300903				
1	-2.154587	1.416859	-0.173910	1	-2.133890	1.425551	-0.075490				
1	1.156339	-1.882853	-0.475777	1	1.258319	-1.716421	-0.865108				
	TS48 CBS-QB3				TS48 CBS-APNO				TS48 G3		
6	-0.262296	1.280085	0.431803	6	-0.244565	1.275203	0.451621	6	-0.247497	1.278497	0.446595
6	-0.908535	-0.000987	0.075971	6	-0.904559	-0.006366	0.067779	6	-0.904455	-0.004874	0.067907
6	0.064447	-1.218545	0.090177	6	0.038222	-1.216293	0.100936	6	0.037876	-1.215919	0.098323
6	1.437784	-0.632514	0.170213	6	1.436254	-0.661535	0.145190	6	1.437174	-0.663642	0.148865
6	1.608822	0.551270	-0.510762	6	1.588098	0.570901	-0.505426	6	1.597223	0.567960	-0.503615
1	1.120971	0.718345	-1.465505	1	1.131267	0.723667	-1.469230	1	1.151551	0.721329	-1.472008
1	2.103731	-0.899528	0.983605	1	2.102051	-0.935739	0.944673	1	2.091737	-0.931811	0.959016
1	-0.169772	-1.891325	0.919991	1	-0.191700	-1.831830	0.965365	1	-0.194459	-1.839091	0.956523
1	-0.133468	-1.776817	-0.832211	1	-0.168036	-1.816313	-0.780693	1	-0.165337	-1.811033	-0.787257
8	-2.061112	-0.094926	-0.286035	8	-2.031245	-0.077726	-0.302181	8	-2.038081	-0.079060	-0.299339

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-0.735369	2.180957	0.050757	1	-0.680765	2.173865	0.048346	1	-0.683379	2.175012	0.039558
1	2.472233	1.182671	-0.326488	1	2.448016	1.189660	-0.311501	1	2.454902	1.186693	-0.302329
1	0.189246	1.369245	1.413709	1	0.128426	1.347030	1.459884	1	0.127705	1.359246	1.452757
	TS49 CBS-QB3				TS49 CBS-APNO				TS49 G3		
6	-0.056376	-1.220200	-0.121183	6	-0.050534	-1.214830	-0.147250	6	-0.052224	-1.216281	-0.144210
6	0.900532	-0.023685	-0.000009	6	0.892072	-0.022631	-0.004587	6	0.890496	-0.023052	-0.004090
6	0.058856	1.263864	0.015334	6	0.069639	1.263912	0.002378	6	0.070428	1.265645	0.005716
6	-1.352213	0.763951	-0.092055	6	-1.348366	0.772696	-0.082731	6	-1.348128	0.775459	-0.083937
6	-1.422608	-0.581221	-0.106929	6	-1.423207	-0.588777	-0.051893	6	-1.424799	-0.588212	-0.055052
1	-2.211608	1.422113	-0.123918	1	-2.199038	1.427786	-0.107947	1	-2.196884	1.432388	-0.112804
1	0.256675	1.826586	0.936124	1	0.280803	1.830422	0.906092	1	0.280848	1.829937	0.910824
1	0.359675	1.916539	-0.812815	1	0.360218	1.887611	-0.839380	1	0.363644	1.892997	-0.832264
8	2.099282	-0.082330	0.068704	8	2.068463	-0.085833	0.084232	8	2.072753	-0.087506	0.080885
1	0.148629	-1.758318	-1.054436	1	0.113896	-1.679295	-1.117358	1	0.115502	-1.689555	-1.109269
1	-2.335381	-1.143240	-0.256496	1	-2.324921	-1.142520	-0.233385	1	-2.324892	-1.141539	-0.244561
1	0.120046	-1.928024	0.693803	1	0.165667	-1.960078	0.608361	1	0.160654	-1.957400	0.616469
1	-1.901446	-0.893270	1.897156	1	-1.781959	-0.939477	1.814264	1	-1.795531	-0.948131	1.813962
	TS50 CBS-QB3				TS50 CBS-APNO				TS50 G3		
6	0.076819	-1.225746	0.100608	6	0.069703	-1.220315	0.097906	6	0.071647	-1.221030	0.097959
6	-0.883240	-0.033542	-0.032007	6	-0.880027	-0.034115	-0.025378	6	-0.878555	-0.034085	-0.025930
6	-0.037521	1.196797	-0.066119	6	-0.050610	1.200295	-0.031722	6	-0.052914	1.200832	-0.032787
6	1.265849	0.853448	-0.137810	6	1.266349	0.855039	-0.144118	6	1.267651	0.856738	-0.143124
6	1.493970	-0.630587	-0.009749	6	1.489264	-0.632367	-0.010885	6	1.491954	-0.631427	-0.010714
1	2.115600	-0.852461	0.865307	1	2.095577	-0.856579	0.862656	1	2.098389	-0.858007	0.861646
1	2.086006	1.553294	-0.249677	1	2.074923	1.552550	-0.263395	1	2.075732	1.554162	-0.262138
1	-0.455676	2.182325	-0.219621	1	-0.470394	2.168075	-0.227752	1	-0.473893	2.166752	-0.234184
8	-2.085317	-0.092306	-0.117633	8	-2.061191	-0.093790	-0.123026	8	-2.065939	-0.096341	-0.121930
1	-0.103834	-1.710891	1.063185	1	-0.108667	-1.707364	1.050379	1	-0.104935	-1.710159	1.049541
1	2.044329	-1.013134	-0.876401	1	2.026988	-1.019128	-0.871602	1	2.029289	-1.018657	-0.871188
1	-0.148600	-1.959917	-0.675242	1	-0.155598	-1.939350	-0.680468	1	-0.151322	-1.941603	-0.679519
1	-0.350541	1.577015	1.903978	1	-0.341369	1.540897	1.799572	1	-0.344448	1.552069	1.798855
	TS51 CBS-QB3				TS51 CBS-APNO				TS51 G3		
6	-0.242085	-1.234301	0.007257	6	-0.264624	-1.197643	-0.104071	6	-0.272274	-1.197367	-0.093201
6	-1.041860	0.061763	0.142698	6	-1.046910	0.102122	-0.006121	6	-1.047238	0.108524	0.006695

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	0.657859	1.458671	0.251530	6	0.668691	1.457735	0.171832	6	0.685881	1.459018	0.178085
6	1.399825	0.501001	-0.395272	6	1.515327	0.446815	-0.299591	6	1.514330	0.440163	-0.309362
6	1.269600	-0.893030	0.152069	6	1.211606	-0.919536	0.257150	6	1.210258	-0.925796	0.248811
1	1.551499	-0.927219	1.209406	1	1.325464	-0.922592	1.338255	1	1.339600	-0.933041	1.327747
1	1.678662	0.631179	-1.436406	1	1.926646	0.517432	-1.293507	1	1.906570	0.507939	-1.310439
1	0.441960	2.415578	-0.212694	1	0.546545	2.379382	-0.371637	1	0.562730	2.382157	-0.361559
1	0.560075	1.445039	1.332632	1	0.463718	1.525828	1.228590	1	0.497629	1.528964	1.237172
8	-2.162632	0.287119	-0.154922	8	-2.192001	0.290788	-0.031984	8	-2.198511	0.298078	-0.042593
1	-0.618025	-1.942907	0.752258	1	-0.738931	-1.948449	0.518824	1	-0.740744	-1.940999	0.542458
1	1.883404	-1.623809	-0.376319	1	1.858656	-1.691145	-0.141742	1	1.848352	-1.699687	-0.159839
1	-0.456556	-1.659436	-0.979191	1	-0.350628	-1.523713	-1.138105	1	-0.371799	-1.537216	-1.120965
	TS52 CBS-QB3				TS52 CBS-APNO				TS52 G3		
6	-0.517719	1.276722	0.179974	6	-0.639995	1.120919	0.159367	6	-0.634496	1.144236	0.155305
6	-1.732228	-0.492297	-0.471293	6	-1.616897	-0.508964	-0.401495	6	-1.600247	-0.501960	-0.411710
6	2.103291	-1.165208	-0.111188	6	2.178923	-1.058700	-0.118776	6	2.142483	-1.077953	-0.122100
6	1.601486	-0.057436	0.424178	6	1.589977	-0.013640	0.426068	6	1.575517	-0.022629	0.429528
6	0.865931	1.014218	-0.334208	6	0.788631	1.017391	-0.322076	6	0.797695	1.030372	-0.313950
1	0.826200	0.763989	-1.399750	1	0.799548	0.799951	-1.385023	1	0.814754	0.824045	-1.378752
1	1.713902	0.114239	1.493970	1	1.673751	0.138530	1.492479	1	1.658065	0.120719	1.496437
1	2.626271	-1.900341	0.490072	1	2.741577	-1.758184	0.474414	1	2.686722	-1.796323	0.464664
1	2.008139	-1.378160	-1.171555	1	2.120369	-1.255221	-1.176406	1	2.084897	-1.265761	-1.180655
8	-2.588442	-0.775022	0.227938	8	-2.544820	-0.776692	0.179729	8	-2.522175	-0.789689	0.184350
1	-1.123040	2.015171	-0.336398	1	-1.247239	1.865842	-0.333694	1	-1.235799	1.887787	-0.345731
1	1.442953	1.953367	-0.268216	1	1.262982	1.991834	-0.195853	1	1.283648	1.996954	-0.174725
1	-0.711458	1.175915	1.243595	1	-0.796259	1.088749	1.227722	1	-0.800598	1.117699	1.221528
	TS53 CBS-QB3				TS53 CBS-APNO				TS53 G3		
6	-0.203543	1.133572	-0.116108	6	-0.197681	1.129564	-0.111123	6	-0.201165	1.129904	-0.110746
6	-1.528355	0.549514	-0.086187	6	-1.528896	0.552398	-0.070531	6	-1.531318	0.552012	-0.068441
6	-1.321869	-0.809755	-0.067594	6	-1.312589	-0.813451	-0.074836	6	-1.312855	-0.816517	-0.074943
8	0.006741	-1.086919	0.021545	8	0.010414	-1.076527	0.026855	8	0.012295	-1.078914	0.027087
6	0.680404	0.111966	-0.021116	6	0.669788	0.106748	-0.019628	6	0.670948	0.108166	-0.019330
1	0.037517	2.183597	-0.155418	1	0.050964	2.169471	-0.152917	1	0.043382	2.171046	-0.154607
1	-2.453636	1.037353	-0.347630	1	-2.436738	1.027932	-0.379533	1	-2.436090	1.025938	-0.390155
6	2.162867	0.037560	0.046762	6	2.154281	0.038041	0.042296	6	2.156852	0.040351	0.042089

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.566168	-0.565239	-0.772513	1	2.543126	-0.556855	-0.778456	1	2.549122	-0.553320	-0.777442
1	2.589686	1.039028	-0.018165	1	2.577072	1.033269	-0.016396	1	2.579715	1.035327	-0.017123
1	2.492454	-0.417475	0.985805	1	2.475864	-0.423401	0.971055	1	2.482834	-0.419479	0.969690
1	-2.037593	0.937945	1.650549	1	-2.029170	0.933083	1.594930	1	-2.040348	0.944054	1.588010
1	-1.985554	-1.656994	-0.049534	1	-1.973849	-1.651081	-0.050593	1	-1.971743	-1.655753	-0.046847
	TS54 CBS-QB3				TS54 CBS-APNO				TS54 G3		
6	1.462020	-0.722940	-0.134631	6	-1.438242	-0.727285	0.196254	6	-1.444191	-0.724211	0.198330
6	1.497559	0.755267	0.093504	6	-1.505522	0.741800	-0.105676	6	-1.505193	0.745664	-0.104914
6	0.020685	1.170371	-0.043481	6	-0.039524	1.157364	0.026251	6	-0.038421	1.155979	0.023307
6	-0.868225	0.216427	-0.041559	6	0.829905	0.173163	0.038748	6	0.831819	0.167288	0.036461
8	0.389586	-1.302040	0.176041	8	-0.381554	-1.287861	-0.247595	8	-0.387104	-1.292227	-0.249360
1	1.832468	1.025701	1.105167	1	-1.853519	0.946521	-1.116008	1	-1.857840	0.951704	-1.113013
1	-0.218281	2.230067	-0.091772	1	0.237125	2.197736	0.065259	1	0.237992	2.196122	0.064169
6	-2.288898	-0.123598	-0.030225	6	2.282101	-0.092343	0.048470	6	2.287270	-0.090954	0.049901
1	-2.522210	-0.741425	0.843202	1	2.564509	-0.643732	-0.842581	1	2.578785	-0.640274	-0.839163
1	-2.923192	0.773143	0.010671	1	2.845960	0.837594	0.072984	1	2.848766	0.839823	0.077078
1	-2.565426	-0.698849	-0.919149	1	2.558431	-0.688730	0.911774	1	2.567002	-0.686092	0.912748
1	2.176916	-1.211787	-0.808806	1	-1.916378	-1.132296	1.081023	1	-1.914052	-1.123069	1.088940
1	2.164188	1.266313	-0.609295	1	-2.156000	1.269597	0.584025	1	-2.151525	1.277007	0.585608
	TS55 CBS-QB3				TS55 CBS-APNO				TS55 G3		
6	2.625010	-0.430855	0.052758	6	2.635265	-0.419118	0.039863	6	2.633952	-0.415325	0.041050
6	1.240745	0.022958	0.221760	6	1.206496	-0.062669	0.203854	6	1.203280	-0.062036	0.208286
6	0.393333	0.890233	-0.272262	6	0.408015	0.902963	-0.219014	6	0.403112	0.903673	-0.223679
6	-1.049702	1.031730	0.147434	6	-1.058276	1.030944	0.110033	6	-1.062077	1.033130	0.110442
6	-1.893964	-0.231061	0.067899	6	-1.886184	-0.234250	0.076360	6	-1.884605	-0.236327	0.080139
8	-1.493107	-1.340527	-0.155647	8	-1.498680	-1.323911	-0.155311	8	-1.489242	-1.328004	-0.159375
1	2.658080	-1.487659	-0.230192	1	2.735539	-1.393029	-0.428746	1	2.738658	-1.391972	-0.420362
1	3.200715	-0.320114	0.977204	1	3.138740	-0.459115	1.001006	1	3.143461	-0.447656	0.999113
1	3.137231	0.144166	-0.734733	1	3.146309	0.314258	-0.582731	1	3.143562	0.312774	-0.588032
1	0.728855	1.558608	-1.074343	1	0.828931	1.689338	-0.834792	1	0.819195	1.684827	-0.847803
1	-1.560260	1.799606	-0.445574	1	-1.538949	1.727065	-0.575122	1	-1.544377	1.729142	-0.573356
1	-1.136093	1.377959	1.188008	1	-1.203531	1.465310	1.100031	1	-1.204019	1.470185	1.099523
1	-2.976203	-0.046380	0.259270	1	-2.949496	-0.059756	0.296269	1	-2.944521	-0.071958	0.308489
	TS56 CBS-QB3				TS56 CBS-APNO				TS56 G3		

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	-2.083606	-0.822732	0.112577	6	-2.076067	-0.923549	0.130360	6	-2.080026	-0.930252	0.130728
6	-1.472510	0.472061	-0.130522	6	-1.595353	0.434094	-0.170818	6	-1.613240	0.434303	-0.170479
6	-0.689296	1.413026	-0.244090	6	-0.770908	1.364278	-0.248647	6	-0.785411	1.366783	-0.247182
6	1.310010	0.893036	0.469032	6	1.220857	0.915546	0.515479	6	1.233162	0.916468	0.516032
6	1.617048	-0.290298	-0.298657	6	1.655210	-0.193900	-0.313281	6	1.665617	-0.186930	-0.315655
8	1.263070	-1.421991	0.008047	8	1.490423	-1.348473	-0.018473	8	1.501940	-1.349274	-0.019329
1	-1.299189	-1.550462	0.350888	1	-1.247811	-1.553687	0.438285	1	-1.245214	-1.557413	0.425488
1	-2.621284	-1.177021	-0.771673	1	-2.538712	-1.364301	-0.745921	1	-2.551480	-1.373249	-0.739592
1	-2.788484	-0.778640	0.947413	1	-2.813285	-0.895648	0.925454	1	-2.807532	-0.915734	0.934936
1	-0.486753	2.426153	-0.515171	1	-0.656367	2.380060	-0.541986	1	-0.671932	2.383533	-0.538048
1	1.012144	0.761957	1.501746	1	0.950134	0.692533	1.531127	1	0.955213	0.692934	1.528715
1	1.807210	1.822219	0.211213	1	1.645952	1.885320	0.323869	1	1.643914	1.891685	0.325481
1	2.181925	-0.118833	-1.238837	1	2.134269	0.064701	-1.261604	1	2.140903	0.070198	-1.263006
	TS57 CBS-QB3				TS57 CBS-APNO				TS57 G3		
6	-2.597238	-0.479726	0.059536	6	-2.624312	-0.463728	0.063341	6	-2.622686	-0.459111	0.064088
6	-1.183788	-0.087782	0.028335	6	-1.179561	-0.133690	0.080625	6	-1.175447	-0.134180	0.083339
6	-0.436899	0.982671	-0.063174	6	-0.445825	0.945959	-0.119191	6	-0.441091	0.948689	-0.122720
6	1.080707	1.043923	-0.099283	6	1.061339	1.042914	-0.049927	6	1.066239	1.044544	-0.047296
6	1.765089	-0.250916	0.304680	6	1.783650	-0.243794	0.296918	6	1.782602	-0.246090	0.297049
8	1.600450	-1.302696	-0.255005	8	1.635764	-1.264540	-0.278100	8	1.622346	-1.270796	-0.279774
1	-2.844008	-1.012541	0.983203	1	-2.946800	-0.845357	1.027125	1	-2.951401	-0.834495	1.028059
1	-2.840836	-1.143996	-0.775620	1	-2.835742	-1.223553	-0.682360	1	-2.837689	-1.222607	-0.676537
1	-3.255759	0.400615	-0.007756	1	-3.218232	0.419030	-0.170131	1	-3.216033	0.421750	-0.175633
1	-0.926282	1.962267	-0.137785	1	-0.949183	1.877572	-0.353982	1	-0.940545	1.879699	-0.363836
1	1.432457	1.857268	0.543815	1	1.342095	1.810357	0.666931	1	1.347519	1.808607	0.672599
1	1.407499	1.285139	-1.120263	1	1.446082	1.367980	-1.016126	1	1.455174	1.375190	-1.009608
1	2.456108	-0.176200	1.173884	1	2.503920	-0.175676	1.122753	1	2.506511	-0.184888	1.116386
	TS58 CBS-QB3				TS58 CBS-APNO				TS58 G3		
6	-2.560386	-0.615720	0.000000	6	-2.550347	-0.612864	0.000003	6	-2.553077	-0.614412	-0.000001
6	-1.153478	-0.155274	0.000000	6	-1.133912	-0.155075	0.000003	6	-1.137324	-0.154304	0.000001
6	-0.571813	1.033874	0.000000	6	-0.563260	1.042051	0.000000	6	-0.563510	1.045007	0.000003
6	0.943160	1.065322	0.000000	6	0.947791	1.060834	0.000004	6	0.948058	1.061095	0.000000
6	1.327316	-0.412182	0.000000	6	1.324082	-0.410937	-0.000001	6	1.323517	-0.412696	0.000006
8	2.395084	-0.927568	-0.000001	8	2.364276	-0.932329	-0.000010	8	2.371258	-0.932691	-0.000008

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-2.774374	-1.231560	0.879573	1	-2.759408	-1.219646	0.875889	1	-2.763522	-1.221552	0.874990
1	-2.774375	-1.231560	-0.879573	1	-2.759405	-1.219653	-0.875879	1	-2.763523	-1.221541	-0.874999
1	-3.263427	0.228937	0.000001	1	-3.234524	0.233005	-0.000002	1	-3.240087	0.228554	0.000005
1	-1.125930	1.972989	0.000001	1	-1.117973	1.967774	-0.000004	1	-1.114763	1.971953	0.000007
1	1.375241	1.557997	0.879721	1	1.372482	1.544316	0.876066	1	1.373476	1.545482	0.874946
1	1.375241	1.557998	-0.879721	1	1.372487	1.544323	-0.876052	1	1.373470	1.545473	-0.874954
1	0.118152	-0.930366	0.000000	1	0.066015	-0.935548	0.000006	1	0.058908	-0.934994	0.000017
	TS59 CBS-QB3				TS59 CBS-APNO				TS59 G3		
6	-2.583099	-0.527405	-0.115478	6	-2.598611	-0.493525	-0.118062	6	-2.598269	-0.494292	-0.119472
6	-1.285358	0.011111	0.396715	6	-1.278945	0.001275	0.395906	6	-1.277466	-0.002830	0.396867
6	-0.420789	0.764216	-0.318472	6	-0.406711	0.745534	-0.314374	6	-0.406950	0.752559	-0.310798
6	0.849052	1.234617	0.170056	6	0.897352	1.170451	0.183328	6	0.897544	1.174608	0.185169
6	2.218255	-0.148039	-0.148567	6	2.164281	-0.131282	-0.181040	6	2.165228	-0.130860	-0.186628
8	1.938479	-1.257060	-0.019251	8	1.938618	-1.229700	-0.013807	8	1.936638	-1.235736	-0.013413
1	-3.426515	-0.175161	0.489878	1	-3.416688	-0.131758	0.500139	1	-3.417023	-0.141655	0.502491
1	-2.601109	-1.622557	-0.064125	1	-2.636236	-1.580015	-0.096116	1	-2.636615	-1.580567	-0.111116
1	-2.761366	-0.233440	-1.152357	1	-2.774747	-0.169239	-1.137926	1	-2.778016	-0.159352	-1.135044
1	-0.662475	0.985585	-1.356419	1	-0.644495	0.997734	-1.335996	1	-0.649225	1.014761	-1.328188
1	0.990944	1.259363	1.248229	1	1.003944	1.190034	1.258635	1	1.006510	1.191671	1.260011
1	1.317439	2.064351	-0.345185	1	1.319882	2.043742	-0.282954	1	1.321577	2.048277	-0.278391
1	-1.033112	-0.228660	1.428464	1	-1.024795	-0.267615	1.410119	1	-1.020834	-0.282350	1.406719
	TS60 CBS-QB3				TS60 CBS-APNO				TS60 G3		
6	-0.139543	1.193132	0.025427	6	-0.136739	1.190993	0.024434	6	-0.137945	1.192584	0.024205
6	-1.475950	0.703194	-0.067057	6	-1.473576	0.705063	-0.064224	6	-1.473661	0.707364	-0.063529
6	-1.378818	-0.660402	-0.125953	6	-1.371391	-0.668222	-0.088280	6	-1.373029	-0.668689	-0.087174
8	-0.064113	-1.032701	-0.127841	8	-0.066059	-1.022107	-0.125643	8	-0.065812	-1.023817	-0.126366
6	0.682614	0.104368	-0.013036	6	0.673831	0.103771	-0.012569	6	0.675732	0.104816	-0.013892
1	0.174043	2.221256	0.113223	1	0.180790	2.210008	0.106097	1	0.177825	2.212445	0.106648
1	-2.389149	1.276432	-0.063688	1	-2.381862	1.270762	-0.061980	1	-2.381223	1.274583	-0.060941
1	-1.879562	-1.085956	1.891196	1	-1.829313	-1.110774	1.739608	1	-1.857489	-1.124870	1.737272
1	-2.089375	-1.442606	-0.327018	1	-2.072260	-1.421592	-0.373639	1	-2.070425	-1.419740	-0.386750
6	2.156954	-0.068244	0.049261	6	2.149813	-0.069236	0.044052	6	2.152615	-0.070009	0.045736
1	2.448616	-0.660839	0.921858	1	2.433720	-0.665156	0.906243	1	2.438141	-0.660178	0.910995
1	2.532135	-0.583928	-0.840085	1	2.510212	-0.576864	-0.845753	1	2.517075	-0.582755	-0.838987

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	2.644651	0.904963	0.115390	1	2.635564	0.896259	0.114090	1	2.640318	0.894655	0.110609
	TS61 CBS-QB3										
6	-0.690254	-0.007416	0.030733								
6	0.138869	1.123293	0.118224								
6	1.476463	0.771140	-0.073064								
6	1.712583	-0.618316	0.083740								
8	-0.120800	-1.159536	-0.092285								
1	-0.247869	2.133227	0.123432								
1	2.197763	1.433002	-0.541049								
6	-2.189329	0.035968	-0.026021								
1	-2.535014	-0.448165	-0.943795								
1	-2.619015	-0.519335	0.813022								
1	-2.561524	1.061219	0.002109								
1	2.403442	-1.133701	-0.581621								
1	1.638622	-1.077967	1.064514								
	TS62 CBS-QB3				TS62 CBS-APNO						
6	0.525464	0.405736	-0.268022	6	-0.634691	0.579685	0.246220				
6	-0.226716	-0.694700	-0.443425	6	0.391045	-0.018779	0.971518				
6	-1.641418	-0.713719	-0.092046	6	1.640870	-0.404661	0.399855				
6	-2.382277	0.286698	0.406085	6	2.101667	-0.053094	-0.837383				
8	0.814239	1.536721	-0.196586	8	-1.140723	1.528777	-0.170072				
1	0.251880	-1.594174	-0.795539	1	0.091661	-0.410882	1.926248				
1	-2.117629	-1.674108	-0.271022	1	2.265455	-1.018365	1.025854				
6	2.516814	-0.666980	0.408309	6	-2.047884	-1.248136	-0.377281				
1	2.750624	0.121099	1.111112	1	-2.067108	-0.976940	-1.418306				
1	2.285708	-1.645466	0.806612	1	-1.562960	-2.173240	-0.119058				
1	2.968393	-0.613430	-0.575246	1	-2.898264	-0.955042	0.214444				
1	-3.436753	0.145622	0.604973	1	3.068779	-0.377814	-1.173512				
1	-1.967329	1.264479	0.626385	1	1.522180	0.551977	-1.512675				
	TS63 CBS-QB3				TS63 CBS-APNO				TS63 G3		
6	-1.718519	-0.067883	-0.012818	6	-1.734754	-0.048217	-0.031313	6	-1.732961	-0.053512	-0.028654
6	-0.674954	0.910584	0.543122	6	-0.673887	0.858003	0.579517	6	-0.679685	0.863953	0.576314
6	0.544795	1.078284	-0.313228	6	0.530899	1.062920	-0.303166	6	0.526878	1.066694	-0.305637
6	1.636654	0.218718	-0.331605	6	1.650729	0.235485	-0.348860	6	1.646375	0.236682	-0.348753

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
8	-1.470669	-1.176428	-0.403254	8	-1.529566	-1.155444	-0.386429	8	-1.512103	-1.162202	-0.389497
1	-0.401589	0.518442	1.532825	1	-0.384293	0.405719	1.524421	1	-0.389022	0.422908	1.526055
1	0.557235	1.938748	-0.973215	1	0.511060	1.921935	-0.951465	1	0.506290	1.923493	-0.956125
6	1.779569	-0.950134	0.386200	6	1.842330	-0.938968	0.364773	6	1.837661	-0.936308	0.369829
1	0.987726	-1.337545	1.014090	1	1.083663	-1.350196	1.003559	1	1.079287	-1.346362	1.008884
1	2.684440	-1.539593	0.311992	1	2.756692	-1.494293	0.263847	1	2.750545	-1.493729	0.272362
1	2.458966	0.506107	-0.983189	1	2.443944	0.546075	-1.009869	1	2.440575	0.544557	-1.009197
1	-2.764365	0.312398	-0.013673	1	-2.742063	0.380820	-0.114009	1	-2.744678	0.358781	-0.103661
1	-1.162331	1.875452	0.707182	1	-1.124381	1.818156	0.809244	1	-1.135781	1.822909	0.799066
	TS64 CBS-QB3										
6	-0.982876	-0.042605	0.037334								
6	0.061462	-1.090928	0.160119								
6	1.370295	-0.831038	0.018220								
6	1.925202	0.536855	-0.146826								
8	-2.146450	-0.332201	-0.183138								
1	-0.306312	-2.107628	0.243689								
1	2.070832	-1.665426	-0.015275								
6	-0.514213	1.378832	0.122389								
1	-1.050589	2.066390	-0.528560								
1	-0.418009	1.749448	1.143700								
1	0.781854	1.261681	-0.205695								
1	2.512117	0.697276	-1.052537								
1	2.422483	0.949169	0.732365								
	TS65 CBS-QB3				TS65 CBS-APNO						
6	0.976422	-0.149377	0.038170	6	1.963898	0.518070	0.671407				
6	-0.232096	-0.479784	0.875943	6	1.486499	-0.286412	-0.504347				
6	-1.494790	-0.230305	0.533003	6	0.235149	-0.573487	-0.811808				
6	-1.961457	0.444864	-0.723137	6	-0.972337	-0.149285	-0.025203				
8	1.411416	-0.953367	-0.795450	6	-1.630222	1.072147	-0.355615				
1	-0.019860	-0.994524	1.810167	1	-2.506085	1.354285	0.199609				
1	-2.279090	-0.551004	1.215524	1	1.147673	0.871518	1.289208				
6	1.632107	1.107598	0.251111	1	2.620352	-0.084081	1.293677				
1	2.509188	1.339816	-0.341808	1	2.538447	1.377385	0.334993				
1	1.278410	1.820801	0.985775	1	2.261046	-0.669633	-1.150406				

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	-1.134458	0.738848	-1.371605	1	0.028993	-1.174799	-1.682963				
1	-2.551975	1.337617	-0.489673	8	-1.414396	-0.858759	0.876563				
1	-2.614660	-0.222606	-1.295319	1	-1.273180	1.709199	-1.143231				
	TS66 CBS-QB3				TS66 CBS-APNO				TS66 G3		
6	-1.336434	0.283531	-0.061830	6	-1.268963	0.224916	-0.065162	6	-1.282131	0.232052	-0.061802
6	0.393236	-1.015376	-0.477449	6	0.344723	-0.910930	-0.591270	6	0.348697	-0.922840	-0.573463
6	1.610499	-0.676631	-0.141174	6	1.572680	-0.630341	-0.194988	6	1.583755	-0.644081	-0.184208
6	2.092523	0.610715	0.467525	6	2.040345	0.583764	0.556336	6	2.061121	0.584730	0.538354
8	-0.947743	1.305688	-0.518672	8	-1.000544	1.239592	-0.602392	8	-0.990660	1.257526	-0.582888
1	-0.085128	-1.861805	-0.946643	1	-0.059841	-1.741414	-1.134042	1	-0.060650	-1.764846	-1.093533
1	2.380248	-1.438196	-0.316695	1	2.329760	-1.367602	-0.432571	1	2.336076	-1.390521	-0.403569
6	-2.158652	-0.566485	0.536650	6	-2.035000	-0.560347	0.664243	6	-2.068778	-0.560457	0.637077
1	-3.095191	-0.161414	0.902379	1	-2.956209	-0.149468	1.033138	1	-2.997331	-0.154277	0.992152
1	-1.918532	-1.601058	0.703137	1	-1.755669	-1.563305	0.899405	1	-1.802007	-1.568425	0.866778
1	1.287611	1.337638	0.554468	1	1.238024	1.286692	0.727818	1	1.264949	1.298754	0.690228
1	2.888084	1.041056	-0.148244	1	2.824039	1.086373	-0.003302	1	2.850571	1.068563	-0.029103
1	2.517819	0.423756	1.458644	1	2.461534	0.289615	1.513734	1	2.477689	0.314118	1.504403
	TS67 CBS-QB3				TS67 CBS-APNO				TS67 G3		
6	-1.078127	0.229594	-0.186645	6	-1.069414	0.210941	-0.125253	6	-1.068383	0.210364	-0.126288
6	-0.046000	-0.754762	-0.567723	6	-0.024159	-0.678826	-0.632165	6	-0.023848	-0.680751	-0.632521
6	1.347354	-0.569766	-0.368295	6	1.375030	-0.482825	-0.446657	6	1.375232	-0.488167	-0.442175
6	1.953020	0.549509	0.412816	6	1.964608	0.580412	0.433583	6	1.966400	0.579049	0.433215
8	-1.266627	1.415223	-0.267931	8	-1.452102	1.316872	-0.245881	8	-1.445737	1.325029	-0.245909
1	-0.353886	-1.549043	-1.237571	1	-0.342726	-1.393990	-1.369656	1	-0.340657	-1.396036	-1.370969
1	2.010149	-1.337432	-0.755012	1	2.031060	-1.252487	-0.816217	1	2.031200	-1.259998	-0.805867
6	-1.320958	-0.871907	0.718915	6	-1.199830	-0.939591	0.751571	6	-1.208629	-0.939813	0.748858
1	-1.913909	-1.727824	0.430999	1	-1.878015	-1.735357	0.508046	1	-1.891069	-1.731877	0.504227
1	-1.121820	-0.732987	1.777217	1	-0.853322	-0.857001	1.766366	1	-0.868340	-0.862296	1.766049
1	1.279354	1.404516	0.494200	1	1.327167	1.455551	0.490706	1	1.326165	1.451414	0.493706
1	2.882509	0.891562	-0.053314	1	2.931488	0.894124	0.053250	1	2.928912	0.897828	0.046533
1	2.218886	0.233426	1.432521	1	2.123761	0.213526	1.448075	1	2.135040	0.216637	1.447061
	TS68 CBS-QB3				TS68 CBS-APNO				TS68 G3		
6	-1.207609	0.154176	-0.175231	6	-1.247090	0.122422	-0.168677	6	-1.250910	0.114349	-0.172689
6	0.036892	-0.951958	-0.473976	6	0.098733	-0.947870	-0.449913	6	0.102862	-0.948684	-0.448654

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
6	1.319323	-0.396152	-0.500719	6	1.368061	-0.340422	-0.525780	6	1.369066	-0.333377	-0.531539
6	1.819058	0.657157	0.433675	6	1.875922	0.716917	0.411797	6	1.876968	0.719966	0.411565
8	-1.456213	1.317678	-0.280076	8	-1.674407	1.206509	-0.271500	8	-1.687397	1.203455	-0.268224
1	-0.204920	-1.731805	-1.186525	1	-0.125224	-1.732948	-1.148604	1	-0.119009	-1.735430	-1.146455
1	1.913244	-0.586758	-1.389501	1	1.914375	-0.485533	-1.442491	1	1.911676	-0.471937	-1.450662
6	-0.929440	-0.903607	0.764033	6	-0.843930	-0.895581	0.774331	6	-0.834908	-0.896075	0.775981
1	-1.596911	-1.760140	0.735834	1	-1.481047	-1.765464	0.814632	1	-1.464295	-1.771124	0.831896
1	-0.557776	-0.669249	1.763615	1	-0.467806	-0.595805	1.742284	1	-0.455103	-0.586978	1.739421
1	1.556596	1.664301	0.073288	1	1.544442	1.708589	0.104020	1	1.499770	1.706559	0.145418
1	2.908106	0.620842	0.517578	1	2.960662	0.724106	0.420075	1	2.959824	0.766453	0.378957
1	1.402019	0.563685	1.439629	1	1.539681	0.562186	1.431536	1	1.587845	0.527749	1.439238
	TS69 CBS-QB3										
6	1.784265	-0.086456	-0.425171								
6	-0.511857	0.885515	0.084484								
6	-1.779127	0.556103	-0.168910								
6	-2.423918	-0.795648	-0.077815								
8	2.913821	-0.279242	-0.145049								
1	-0.221706	1.925663	-0.038432								
1	-2.443453	1.359351	-0.480482								
6	0.589781	-0.028311	0.539522								
1	0.986691	0.272507	1.518320								
1	0.252589	-1.065563	0.627477								
1	-2.845669	-1.084868	-1.046457								
1	-3.257303	-0.777191	0.632941								
1	-1.736587	-1.583177	0.234364								
	TS70 CBS-QB3				TS70 CBS-APNO				TS70 G3		
6	1.997500	-0.118289	0.097655	6	1.948634	-0.121953	0.055853	6	1.950568	-0.119289	0.049411
6	-0.478966	1.089098	-0.399602	6	-0.446999	1.097932	-0.374995	6	-0.447231	1.102600	-0.373726
6	-1.486000	0.188520	-0.498647	6	-1.484258	0.237473	-0.479190	6	-1.485035	0.237270	-0.479069
6	-1.774441	-0.950157	0.428645	6	-1.789999	-0.934985	0.407263	6	-1.787071	-0.937162	0.407206
8	1.728311	-1.124438	-0.392561	8	1.685823	-1.131801	-0.387703	8	1.680800	-1.140567	-0.383479
1	-0.397469	1.832339	-1.188446	1	-0.361534	1.865784	-1.126330	1	-0.363682	1.871178	-1.123928
1	-2.165602	0.291283	-1.340884	1	-2.176929	0.399421	-1.289609	1	-2.179109	0.397525	-1.287746
6	0.549234	1.121647	0.607865	6	0.626567	1.051059	0.613341	6	0.627295	1.057106	0.611847

Table 16: Cartesian coordinates of all transition state structures.

At. No.	X	Y	Z	At. No.	X	Y	Z	At. No.	X	Y	Z
1	1.123915	2.034827	0.702794	1	1.170181	1.970637	0.744300	1	1.172034	1.975764	0.742503
1	0.355757	0.640196	1.562425	1	0.399822	0.582270	1.558530	1	0.402406	0.588889	1.557489
1	-1.658056	-1.907257	-0.092767	1	-1.758442	-1.856569	-0.167984	1	-1.754372	-1.859688	-0.165795
1	-2.810934	-0.911085	0.782439	1	-2.791523	-0.846986	0.821347	1	-2.787203	-0.854051	0.824700
1	-1.118059	-0.969706	1.299432	1	-1.091832	-1.037310	1.227744	1	-1.087636	-1.038235	1.226589

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